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FISCAL YEAR 2003 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

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NOTICE

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PREFACE

This report summarizes the Fiscal Year 2003 research and operational activities of the Atmospheric Sciences Modeling Division (ASMD), Air Resources Laboratory, National Oceanic and Atmospheric Administration, working under the Memorandum of Understanding and Memorandum of Agreement between the U.S. Department of Commerce (DoC) and U.S. Environmental Protection Agency (EPA) through long-term Interagency Agreements DW13938483 and DW13948634 between EPA and the National Oceanic and Atmospheric Administration (NOAA), U.S. Department of Commerce. The summary includes descriptions of research and operational efforts in air pollution meteorology, atmospheric modeling, air quality model development and evaluation, and air pollution abatement and compliance programs aimed at improving the Nation's air quality.

Established in 1955, the Division serves as the vehicle for implementing the interagency collaboration on atmospheric research efforts. ASMD conducts research activities in-house and through contract and cooperative agreements. ASMD also provides technical information, forecasting support, and consultation on the meteorological and air quality modeling aspects of air quality management to various EPA offices, including the Office of Air Quality Planning and Standards, and to state/local agencies. To provide these services, the Division is organized into three research Branches and an operational Branch: Atmospheric Model Development Branch, Model Evaluation and Applications Research Branch, Air-Surface Processes Modeling Branch, and Air Policy Support Branch. The report is organized by major program themes reflecting the Division strategic plan and supporting NOAA's mission.

Any inquiries on the research or support activities outlined in this report should be sent to the Director, NOAA, Atmospheric Sciences Modeling Division (E243-02), U.S. Environmental Protection Agency, 109 T. W. Alexander Drive, Research Triangle Drive, NC 27711.

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ABSTRACT. During Fiscal Year 2003, the NOAA Atmospheric Sciences Modeling Division's work on meteorological and air quality modeling, and policy guidance was accomplished in accordance with the memorandum signed by the Department of Commerce and the U.S. Environmental Protection Agency (EPA). This ranged from research studies and model applications to the provision of advice and guidance in developing programs for improving the Nation's air quality. Research efforts emphasized the development, evaluation, and application of meteorological and air quality models. Among the research studies and results were the release in September 2003 of the latest version of the Community Multiscale Air Quality (CMAQ) modeling system; continued development and improvement of CMAQ and its modules; completion of the wind tunnel modeling study of the estimation and characterization of the dispersion of particulate matter from the World Trade Center recovery site after September 11, 2001; development and evaluation of fine or neighborhood-scale air quality models; development of techniques for model evaluation; development of an updated version of the Biogenic Emissions Inventory System; initiation of a study to model the smoke emissions from prescribed and wildfires; and development of the Eta-CMAQ modeling system for use in air quality forecasting.

1. INTRODUCTION

In Fiscal Year 2003, the Atmospheric Sciences Modeling Division (ASMD) continued its commitment for providing goal-oriented, high quality research and development, and operational support of the missions of NOAA and EPA. Using an interdisciplinary approach emphasizing integration and partnership with EPA and public and private research communities, the Division's primary efforts focused on studying processes affecting the dispersion of atmospheric pollutants through numerical modeling as well as physical modeling; and developing and evaluating meteorological and air quality models on all temporal and spatial scales. The research products developed by the Division are transferred to the public and private national and international user communities.

Division research is focused on five areas: new developments in air quality modeling; global climate change and its impact on regional air quality; multimedia modeling; data management and analysis; and air quality forecasting. The Division is organized to respond effectively to these research directions as more fully described in the following sections of the report. A new version of the Community Multiscale Air Quality (CMAQ) modeling system, incorporating the latest developments in state-of-science in modeling ozone and fine particles, was released in August 2003. Research continued to develop and apply statistical techniques for evaluating air quality model performance in reproducing the spatial and temporal features embedded in the observational data. In collaboration with the National Weather Service and Oceanic and Atmospheric Research, CMAQ was linked with the NOAA meteorological model, Eta, for the preparation of national air quality forecasts by the National Weather Service. Initial forecasts are for ozone. To improve the simulation of the transport and fate of airborne agents in the near-field, a scale model of Lower Manhattan was used in the wind tunnel to study the impact of pollutant release from ground zero. These studies will help improve the predictions using computational fluid dynamics models and mesoscale models to quantify the adverse impacts from the collapse of the World Trade Center and other near-field events.

2. PROGRAM REVIEW

2.1 Atmospheric Model Development

This research is aimed at providing state-of-science air quality models and guidance for their use in the implementation of National Ambient Air Quality Standards (NAAQS) for ozone and fine particulate matter ($PM_{2.5}$). The principal effort is to develop and improve the Models-3/CMAQ modeling system, a multiscale and multi-pollutant chemistry-transport model (CTM). Specific research components include: meteorological modeling, land-surface and planetary boundary layer (PBL) modeling, emissions modeling, gas-phase chemical mechanisms and solvers, aerosol representations in grid-based air quality models, plume-in-grid treatment for large elevated sources of pollution, CMAQ code integration and efficiencies, and air quality forecasting.

The objectives of this research program are to continuously develop and improve the mesoscale (regional through urban scale) air quality simulation models, including CMAQ, as air quality management and NAAQS implementation tools. The CMAQ CTM includes the necessary critical science process modules for handling atmospheric transport, deposition, cloud mixing, emissions, gas- and aqueous-phase chemical transformation processes, and aerosol dynamics and atmospheric chemistry. Research is conducted to develop and test appropriate chemical and physical mechanisms, improve the accuracy of emissions and dry deposition algorithms, and to develop and advance state-of-science meteorology models and contributing process parameterizations.

By design, CMAQ is expected to be used by both scientists and policy makers for assessment activities, research module developments, and detailed model evaluation studies. Scientists can thus incorporate additional air quality science process modules into the system. A generalized coordinate approach used in CMAQ allows the CMAQ CTM to be configured dynamically consistent with the driver meteorology model. Tested model configurations can be established for use by the policy community to develop and analyze implementation strategies for air quality management. CMAQ supports the vision of "one atmosphere" approach to air quality modeling. It is capable of concurrently simulating concentrations of oxidants, fine particles, visibility degradation, air toxins, and acidic and nutrient deposition and loadings to ecosystems at urban and regional scales. As the understanding of atmospheric processes, input data, and model formulations and parameterizations improve, it will be essential to continue to upgrade or provide science options through future releases of CMAQ. Therefore, activities that facilitate the maintenance and science process evolution within CMAQ will be required. The work described below includes additional model development and testing leading to the September 2003 release, as well as future releases, of the CMAQ modeling system.

2.1.1 Meteorological Modeling for CMAQ Applications

The Fifth-Generation Pennsylvania State University (PSU)/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) is the primary tool for providing meteorological input for Models-3/CMAQ. MM5 is widely used to generate meteorological characterizations of the atmosphere throughout the air-quality modeling community. For Models-3/CMAQ, MM5 is applied to case studies (episodic, seasonal, and annual) at a variety of spatial scales using a series of one-way nested domains. MM5 is run retrospectively using four-dimensional data assimilation (FDDA) for a dynamic analysis of the simulation period. The output represents a dynamically-consistent multiscale meteorology simulation for various horizontal grid spacings ranging from continental to urban scales. The MM5 output is ultimately used in the Sparse Matrix Operator Kernel Emission (SMOKE)©[1] (emissions) and CMAQ (chemistry) modules to describe the atmospheric state variables and the planetary boundary layer characteristics.

Several projects were underway during FY-2003 using MM5 to support Models-3/CMAQ applications. MM5 version 3 release 6 (MM5v3.6) was made available to the modeling community by NCAR in December 2002. MM5v3.6 included updates to the Pleim-Xiu land-surface model (Xiu and Pleim, 2001). During FY-2003, MM5v3.6 was tailored for air quality applications with minor modifications to the science algorithms and parameters, and it was used in various research projects.

During FY-2003, MM5 was used to drive CMAQ for a 10-week summer modeling period based on the photochemical field studies from the Southern Oxidants Study (SOS) in Nashville and Atlanta during the summer of 1999. Meteorological and chemical observations were made in Nashville during June and July 1999, and chemical observations were made in Atlanta during August 1999. The modeling of SOS 1999 consisted of a common domain with 32-km horizontal grid spacing and separate 8-km and 2-km domains over each of the focal cities. Evaluation

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included comparison to surface observations, radar wind profilers, and surface flux measurements. Some evaluation results are presented in Pleim and Xiu (2003).

A series of 32, 8, and 2 km grids of nested simulations for the spring and summer of 2002 were made for the Bay Regional Atmospheric Chemistry Experiment (BRACE) of Tampa , Florida. These runs will support CMAQ simulations that will be evaluated against a variety of experimental field data for both meteorology and air chemistry. Continental-scale runs for January and February of 2002 were also made to support development and evaluation of the latest release of CMAQ. These runs focused on nitrate aerosols.

During the summer of FY-2003, the new version of the Weather Research and Forecast (WRF) model was run in-house on a daily basis. WRF is expected to be the next-generation meteorology model that will include many of the features currently in MM5. It is also attractive for air-quality modeling applications because it contains mass-conserving equations unlike MM5. The initial version of the model evaluation tool was used to assess the error and biases of the model. Plans are to use the WRF data in the CMAQ model and compare against traditional MM5-CMAQ applications.

2.1.2 Linking Meteorology and Chemistry Models for Research Applications

The Meteorology-Chemistry Interface Processor (MCIP) creates the off-line linkage between meteorological models and CMAQ. It is essential that MCIP is compatible with upgrades to the meteorological models that are used by CMAQ to preserve numerical and physical consistency between the meteorology and chemistry models. In FY-2003, MCIP was upgraded twice. For MCIP version 2.1 (MCIPv2.1), several important software errors were identified and corrected; these errors were part of the original MCIP code. A major error was identified in the layer collapsing section; the component wind fields that are used for the chemistry transport were improperly set for the CMAQ vertical structure. The largest impacts to the CMAQ simulation from that correction are expected when the number of vertical layers is significantly reduced from the meteorology to the chemistry simulations, when layer collapsing begins near the surface, when there is strong vertical shear, and when the wind speed is high. In addition, algorithmic errors were corrected for the translation of winds from the Arakawa-B used by MM5 to the Arakawa-C grid used by CMAQ, and for the hydrostatic and non-hydrostatic calculations of the vertical velocity field used by CMAQ. MCIPv2.1 was released to the public in March 2003.

The primary focus of MCIPv2.2 was the improvement of the calculation of dry deposition velocities with an emphasis on winter simulations. Several changes were made to both the M3Dry and RADMDry dry deposition schemes to include the effects of snow cover and the addition of new chemical species. Also, several files that were routinely generated by MCIP but never used were eliminated, and the overall output size was reduced by 17%. MCIPv2.2 was designed to be a companion to the CMAQ summer 2003 release, and MCIPv2.2 was released to the public in June 2003.

2.1.3 Land Surface and Planetary Boundary Layer Modeling

Realistic simulation of land surface and PBL processes are critically important for both meteorology and air quality modeling. Interactions between surface characterization, surface fluxes, and PBL processes are very tightly coupled. In addition, surface fluxes and PBL mixing of chemical constituents closely follow the meteorological processes. Hence, work involves both the meteorology and chemical transport models to develop realistic and consistent modeling of surface and PBL processes.

For many years, this effort has focused on the development, testing, and implementation of the Pleim Xiu land surface model (PX LSM) (Xiu and Pleim, 2001) in the MM5 and the M3Dry dry deposition model in CMAQ. The M3Dry scheme is linked to the PX LSM by use of the canopy bulk stomatal resistance and aerodynamic resistance directly from the PX LSM. These modules are in public releases of both MM5 and CMAQ, providing the capability of using the same PBL scheme for both meteorological and chemical species. The Asymmetric Convective Model (ACM) is part of the PX LSM implemented in MM5 and was added to CMAQ in the 2002 release.

In FY-2003, the data-assimilation scheme in PX LSM was analyzed and evaluated against SOS 1999 field experiment data. This scheme involves Newtonian nudging of surface and root-zone soil moisture according to model biases in 2-m air temperature and relative humidity. The coupling coefficients, nudging strength, are parameterized to nudge most strongly when the influence of soil moisture on the surface layer air is strongest. Sensitivity tests confirm the value of this scheme in improving temperature and surface flux simulations (Pleim and Xiu, 2003).

2.1.4 High-Resolution Sea Surface Temperature Initialization for Meteorological Models

The initial version of a sea surface temperature (SST) processing utility for MM5 was developed in FY-2003. The main reasoning behind this development is that typically MM5 uses coarse, 32 km or more, gridded SST data interpolated from larger scale models. In coastal areas, the sea temperature is one of the most dominating factors influencing the boundary-layer meteorology so it is import to resolve it to the grid scale of the model. The first MM5 simulation in this study is focused over Tampa Bay, Florida (April 20 - June 7, 2002). It is expected that the more detailed SST will improve the simulated coastal meteorology. A similar approach will be applied to a 1-km grid-model simulation over the Houston area. Additionally, real-time simulations with and without the high-resolution SST are being compiled during 2004. Figure 1 displays a sample of the SST data in the Eastern Gulf of Mexico, near Florida. All simulations will be evaluated with observations to provide a better idea to what extent the more detail SST improves the representation of the actual atmosphere.

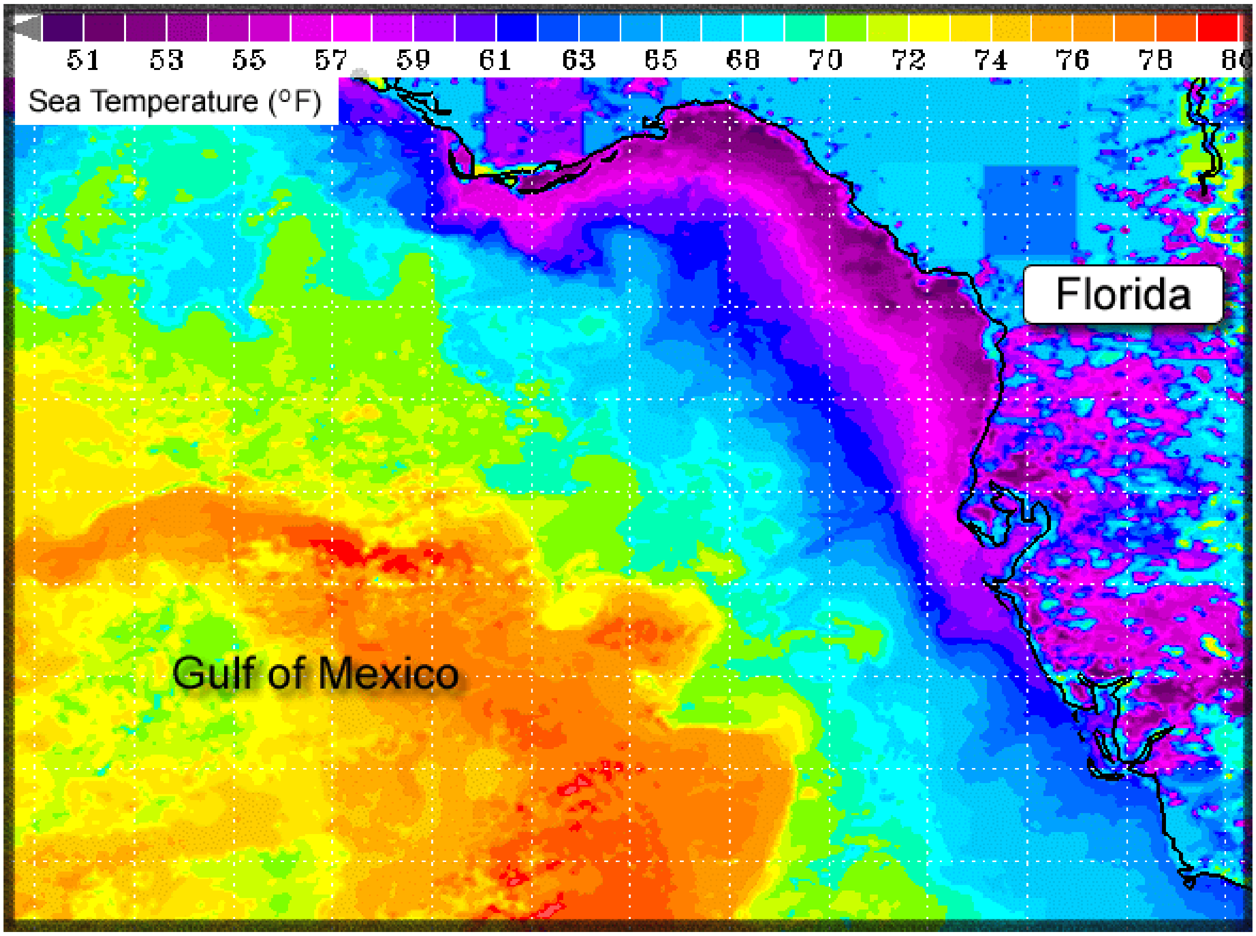

Figure 1. Gridded sea surface temperature (°F) in the Eastern Gulf of Mexico.

2.1.5 Anthropogenic Emissions

The SMOKE© modeling system (www.cep.unc.edu/empd/products/smoke/index.shtml) was enhanced to version 2.0. Version 2.0 explicitly allows use of criteria and/or toxic volatile organic compound (VOC) emission inventories from the EPA National Emission Inventory and National Toxic Emission Inventory. Speciation files were created for the Carbon Bond-IV (CB-IV) lumped-species mechanism, which allow substitution of toxic VOCs for VOC species derived from the VOCs criteria inventory. The control strategy input format and design were improved, *e.g.*, control strategies can include changes in the reactivity of emitted species. This is important when industrial processes are changed. In addition, a variety of software bugs were fixed. Development of SMOKE© is continuing with the gradual development by several entities for modeling of wild fire emissions (ASMD and U.S. Forest Service), and alternative land-cover and wildfire emissions (EPA Office of Air Quality and Planning Standards (OAQPS)). Most data input format features needed by SMOKE are included in the system, with the exception of spatial gridding of input files and spatial surrogates. To meet this need, preparation and testing of the spatial allocator tool of the Multimedia Integrated Modeling System (MIMS) is near completion. The spatial allocator requires only grid definitions and Geographic Information System (GIS) shape files for spatial surrogates.

2.1.6 Biogenic Emissions

Introduced in 1988, the Biogenic Emissions Inventory System (BEIS) provides hourly, gridded estimates of biogenic VOC and soil NO emissions to such regional air quality models as CMAQ. During FY-2003, BEIS was upgraded from version 3.09 to version 3.12 (Pierce *et al.*, 2003). BEIS3.12 includes emission factors for 34 chemical species, including 14 specific monoterpenes, methanol, and methyl-butenol (MBO). While previous versions used solar radiation to modulate emissions of isoprene, BEIS3.12 has extended its use of solar radiation adjustments to include methanol and MBO. The soil NO algorithm has been enhanced to account for soil temperature, fertilizer application schedules, rainfall, and crop growth. The new soil NO algorithm is the most significant change in BEIS compared to BEIS3.09. As shown below in Figure 2, soil NO emissions with BEIS3.12 peak during the spring, soon after most fertilizer applications and during periods of frequent rainfall. Soil NO emissions for this 2001 simulation averaged 30% higher than with BEIS3.09. The Division plans to assess this impact of the new biogenic emission estimates with the CMAQ model during FY-2004. If testing with BEIS3.12 proves successful, BEIS3.12 will be packaged as part of the SMOKE system and released to the public..

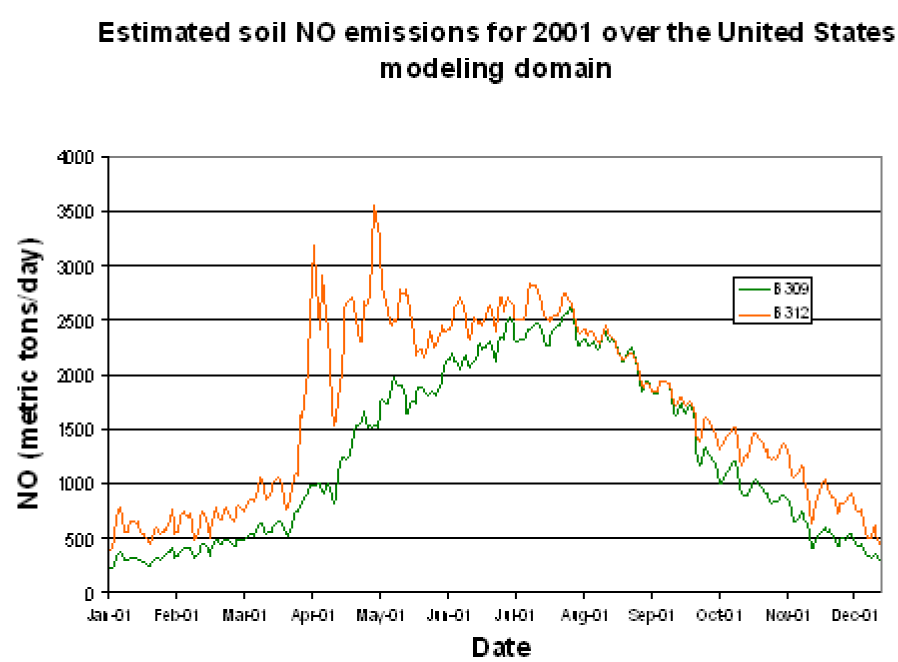

Figure 2. Estimated soil NO emissions using two versions of BEIS model.

2.1.7 Modeling Smoke Emissions from Fires

A prototype, stand-alone emissions processor was developed to model smoke from fires (prescribed and wildfires). The goal of this project is to build a tool to generate emissions from forest burning for use in regional air quality modeling with the following characteristics:

- horizontal scale from regional to national with grid spacings ranging from 1 km to 36 km;
- temporal resolution ranging from hourly to multi-year;
- chemical species, including all NAAQS and visibility components and their precursors; and
- accuracy equivalent to other emissions estimates.

This prototype system, consists of a set of processors based on state-of-science algorithms developed primarily by the U.S. Forest Service. This development was a cooperative effort with the National Park Service and included principals at the Cooperative Institute for Research in the Atmosphere, Colorado State University, Fort Collins, Colorado. This project will serve to facilitate the use of Models-3/CMAQ to develop science-based strategic plans for dealing with smoke emission management issues and interstate transport affecting regional haze, $PM_{2.5}$, PM_{10}, and ozone. The effort to develop the smoke emission processor will involve introducing several major components, including:

- a system to identify fire boundaries determined from GIS coverage;
- fuel models to introduce vegetation coverage and fuel loading data associated with the fires;
- a fuel moisture model;
- a fire generation processor based on spatial coverage of historical wildfire;
- a processor based on the U.S. Forest Service Consume[2] model for determining fire behavior or biomass consumption; and
- a processor for computing plume rise and providing emissions profiles for speciated wildfire emission pollutants.

The plan is to collaborate with the U.S. Forest Service and EPA's OAQPS to update and refine the prototype fire model and link it with the SMOKE© emission modeling system for use with CMAQ.

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[2]A fuel consumption model, which predicts total smoldering fuel consumption during wildfires.

2.1.8 Fugitive Dust Modeling

Windblown and fugitive dust from on- and off-road activities, industrial and construction activities, and agricultural tillage practices are sources of PM_{10} in the atmosphere. Hourly contributions from these sources are not incorporated in CMAQ because of a lack of an acceptable emission processing system to models these fluxes. Algorithms for estimating the emissions of windblown and fugitive dust involve complex atmospheric processes and linkages with spatially and temporally variable land surfaces, soil types, and soil conditions.

Initial development of a prototype windblown dust model to be used in CMAQ at 36-km horizontal cell sizes was completed and work begun on its application to human-caused dust generating activities, including dust from unpaved roads, construction sites, and agricultural activities. The resulting applications will be included as modules in the SMOKE© emission modeling system. The basis for the wind blown dust formulation is derived from use of threshold friction velocity parameterizations, and incorporation of gridded databases prepared with information on soil types, surface soil moisture content, weather, and vegetation type and coverages.

2.1.9 Implementation and Testing of New and Refined Chemical Mechanisms and Chemical Solvers in CMAQ

The treatment of atmospheric, gas-phase chemistry is a critical component of the CMAQ modeling system. The ability of CMAQ to accurately predict ambient concentrations of trace gases in the atmosphere is fundamentally dependent upon the validity of the gas-phase chemical interactions and transformations contained in the chemical mechanism that is used in CMAQ. Accurate representation of gas-phase chemistry is also vital for the simulation of such other important atmospheric processes as the formation of aerosols, the chemical transformations taking place in the liquid phase, and the deposition of air contaminants to land and water surfaces. Commensurate with the need for an accurate chemistry representation is the need for gas-phase chemistry solution techniques that are both highly accurate and computationally efficient. Since numerical solution techniques that have been used historically consume about 50 to 75 percent of the computer time required for model simulations, any substantial computational efficiencies that can be gained will significantly lower the computational requirements of the model. Therefore, the underlying objectives of this research effort are twofold: (1) to improve and enhance the representation of atmospheric gas-phase chemistry in CMAQ by refining existing chemical mechanisms, by adding new chemical mechanisms, and by investigating new approaches for increasing chemical information in the model, and (2) to reduce computer time required to simulate gas-phase chemistry by enhancing the computational efficiency of existing solvers, by investigating new approaches that can be used in conjunction with existing solvers to lower computational requirements without sacrificing the numerical accuracy, and by testing and evaluating new chemistry solver algorithms. The results of this work will help improve the scientific integrity of CMAQ by incorporating new scientific knowledge in atmospheric chemistry, and will increase the practicality of using CMAQ as a modeling tool in regulatory/operational modeling applications by lowering the computational burden.

During FY-2003, a variant of the Modified Euler Backward Iterative (MEBI) solver was added to the array of gas-phase chemistry solvers in CMAQ. The new solver utilizes a formulation similar to the Euler Backward Iterative (EBI) solver originally published by Hertel *et al.* (1993). It is comparable to the existing MEBI approach, except that numerical solutions for two groups of mechanism species are replaced by analytical expressions that provide approximate solutions. Although this approach is somewhat less general than the numerical scheme used in MEBI, computational efficiency is improved with minimal loss in accuracy. Thus far, the new EBI solver was developed for the CB-IV chemical mechanism where tests conducted with CMAQ have shown it to be about two times faster than its MEBI analog. It was included in the latest CMAQ public release, and it also is being used in the air quality forecasting version of CMAQ. The use of the same approach for the SAPRC99 chemical mechanism is being tested, with an anticipated release in FY-2004.

2.1.10 Aerosol Mechanism Improvements in CMAQ

The CMAQ aerosol module was revised to improve predictions of aerosol-phase nitrate and secondary organic aerosol concentrations. Evaluations of the 2002 CMAQ release revealed large overpredictions in the wintertime aerosol nitrate concentrations and year-round organic carbon concentrations. To mitigate the nitrate overprediction, extensive analyses of the available ambient data and relevant scientific literature were conducted. Ultimately, the heterogeneous reaction probability of gaseous dinitrogen pentoxide with liquid water was modified to allow the reaction probability to be computed as a function of the aerosol chemical composition instead of using a fixed value. This modification is based on experimental evidence suggesting that the heterogeneous reaction is inhibited by the presence of nitrate in the aerosol phase, and follows the implementation of Riemer *et al.* (2003). In addition, the production pathway of nitric acid via gas-phase hydrolysis of dinitrogen pentoxide has been removed, based on the work of Jacob (2000). As a result of these modifications, the CMAQ overpredictions of wintertime nitrate were largely mitigated.

The overpredictions of organic carbon concentrations in the 2002 release of CMAQ were largely due to a model assumption that restricted semi-volatile organic compounds (SVOC) evaporation. Several changes were required to relax this assumption in the 2003 CMAQ public release. In addition, various corrections were made to the SVOC production rates to account more accurately for the specific compounds within lumped compound groups that yield secondary organic aerosol (SOA). For example, the entire ARO1 lumped group in SAPRC99 is treated as an SOA precursor although it includes benzene, which is not an SOA precursor. Therefore, the production rate of SVOCs arising from the oxidation of ARO1 must be scaled down to account for the amount of benzene that is lumped with ARO1. Adjustments analogous to this one were made to decrease the excess SOA production that arises artificially from compound lumping.

2.1.11 Plume-in-Grid Modeling

The plume-in-grid (PinG) approach within the CMAQ modeling system provides for the subgrid scale treatment of the physical and chemical processes governing gaseous pollutants and aerosol species in isolated, major-point source plumes within an Eulerian grid framework. By applying a Lagrangian approach, the CMAQ/PinG treats the horizontal and vertical growth of a plume section in a gradual, real-world manner due to turbulence and wind shear processes, which is in contrast to the instantaneous mixing of point emissions into the entire grid cell volume in the traditional Eulerian modeling method. The key modeling algorithms are a plume dynamics model (PDM) and a Lagrangian reactive plume model (PinG module), which are designed to simulate the relevant plume processes at the proper spatial and temporal scales for CMAQ regional model domains with a typical grid spacing above about 10 km. The PinG treatment was designed to simulate multiple point-source plumes. A continuous plume is represented by a series of plume sections released at 1-hour intervals and each horizontal plume cross-section is internally resolved by a set of attached plume cells. The PinG module is fully integrated into the CMAQ grid model, and it is exercised concurrently during a simulation in order to use grid cell concentrations as boundary conditions at each edge of a plume section. An important feedback occurs when a plume section reaches the model grid cell size as the subgrid plume treatment ceases and plume concentrations are incorporated into the Eulerian grid system. A full description of the capabilities of the CMAQ/PinG modeling treatment and its technical formulation were described by Gillani and Godowitch (1999).

During FY-2003, an updated AE3 aerosol algorithm was included in the PinG module to simulate aerosol species and $PM_{2.5}$ along with gas-phase pollutant species in the subgrid plumes. Additional code revisions were also undertaken to permit a more frequent plume release rate than the previous hourly default interval. CMAQ/PinG test simulations were successfully completed on various computational platforms with single processors and multi-processors. Preliminary results of modeling aerosols in PinG presented by Godowitch (2002) revealed differences in aerosol sulfate (SO_4) concentrations among the high NO_x and SO_2 point sources. For point sources with comparable SO_2 emissions, greater sulfate formation occurred in those plumes exhibiting a lower NO_x emission rate. These PinG results also appeared to agree with emerging observed plume aerosol data. In addition, separate CMAQ model simulations were conducted with PinG and excluding the PinG module using existing emission and meteorology data sets from a summer period for a large eastern United States domain with a 36-km grid cell size. There were 77 high-emitting NO_x and SO_2 point sources in the modeling domain simulated with the PinG approach. Comparisons of modeled gaseous and aerosol species against surface monitoring network data have commenced. So far, analyses of peak and hourly ozone concentrations reveal that the CTM/PinG results displayed better agreement and less bias than the CTM/NoPinG results, particularly in model areas where numerous large point sources exist. Additional model runs are planned for a different summer experimental period when observed plume data collected by various airborne platforms are available. Evaluation results with the CTM/PinG are expected during FY-2004. Further sensitivity test runs will be performed to assess computational times and to investigate the impact on oxidant and aerosol species concentrations using different chemical mechanisms (*e.g.*, CB-IV, SAPRC) and different chemistry solvers (*e.g.*, Gear, Euler Backward Interative solver) available in the CMAQ modeling system.

2.1.12 CMAQ Code Integration and 2003 Release

CMAQ was extensively revised in 2003. Changes include updated science, corrected implementations, efficiency enhancements, and bug fixes. The biggest changes involve aerosol modeling, particularly nitrate aerosols and SOA. Nitrate modeling was updated so it is consistent with the most recent literature and the SOA implementation was corrected to allow for reversible semi-volatility. These changes resulted in substantially lower concentrations of both aerosol nitrates and SOA. Minor changes were made to aqueous processes and dry deposition.

There were major modifications to improve model efficiency. A new fast gas phase chemistry solver, known as the Euler Backward Iterative (EBI) scheme, was developed for the CB-IV mechanism. Also, some of the fastest reacting species have been dropped from the transport processes. The time step for operator splitting has been revised to allow different advective time steps by vertical layer.

Note that other components of the CMAQ system as SMOKE© and MCIP were also revised recently. Therefore, MCIPv2.2 needs to be used for CMAQ modeling. The latest version of CMAQ (September 2003) features several major changes:

a. Scripts to build and run CMAQ for MPICH[3] Linux clusters; and
b. Incorporated the I/O API version 2.2.
c. Modified the treatment of secondary organic aerosol (SOA) formation:
    i. The SOA algorithm was modified to make the gas-particle partitioning of semi-volatiles reversible;
    ii. Eliminated SOA production from anthropogenic alkenes;
    iii. Adjusted yields of semi-volatiles from alkanes and aromatics to account for emissions of non-SOA producers being lumped with those from SOA-producers; and
    iv. Modified gas-phase monoterpene reactions rates in RADM2 and CB-IV.
d. Modified the heterogeneous N_2O_5 reaction probability;
e. Added an EBI gas-phase chemistry solver for the CB-IV family of chemical mechanism;
f. Implemented layer-dependent horizontal advection time-stepping; and
g. Changed the order of the time splitting science processes to: vertical diffusion–> advection–> mass-adjustment–> horizontal diffusion–> clouds–> chemistry–> aerosols.

[3]MPICH is a freely available, portable implementation of MPI, the Standard for message-passing libraries.

h. Updated all gas-phase chemical mechanisms (CB-IV, RADM2, SAPRC):
   i. New deposition velocity surrogates;
   ii. New cloud scavenging surrogates;
   iii. Zeroed reaction rate constant for $N_2O_5 + H_2O$ -> $2HNO_3$ in all AERO3 mechanisms; and
   iv. For CB-IV, eliminated advection and diffusion of fast-reacting species.
i. Cloud enhancements/updates:
   i. Modified to use effective Henry's Law constant for scavenging;
   ii. Updated and added new coefficients to the Henry's Law constant table;
   iii. Revised the timestep calculation in the aqueous chemistry subroutine; and
   iv. Updated the coarse-mode aerosol number washout.
j. Other enhancements and bug fixes:
   i. Modifications of the vertical diffusion module were made to improve data locality to speed up computation;
   ii. For the heterogeneous N_2O_5 reaction in the aerosol module, an error was corrected in the concentration units for calculating the HNO_3 yield, and the rate constant calculation for this reaction was changed to use effective radius instead of diameter;
   iii. An error in the contribution of N_2O_5 to total initial HNO_3 was corrected in the cloud module;
   iv. Changed the units for aerosol for vertical diffusion to molar mixing ratio instead of mass density concentration; and
   v. Updated the minimum aerosol concentration array and bug fix in coarse-mode aerosol standard deviation in the aerosol dry deposition subroutine.

2.1.13 Development and Testing of an Air Quality Forecast Model

As part of a joint NOAA-EPA project on air quality forecasting, an optimized version of the CMAQ model has being linked with the NOAA/National Weather Service (NWS) mesoscale Eta meteorological model. ASMD is collaborating with the NWS National Center for Environmental Prediction (NCEP) to produce an initial air quality forecast capability for the nation. Appropriate linkage software to drive CMAQ with the Eta model output has been developed and tested. Other objectives of this work are to make significant improvements in the computational performance of the CMAQ model so it can be used effectively in an operational forecasting environment.

During FY-2003, the initial Eta-CMAQ system was constructed and tested, and used to make daily forecasts for ozone in the northeast United States from July through September. The CMAQ model was run twice daily at NCEP to produce forecast guidance. The principal CMAQ model run was driven by the 12Z Eta forecast. CMAQ simulations were made for 48-hour duration, and were available by 1:30 p.m. EDT. A 30-hour update CMAQ simulation was run using the 06Z Eta forecast, and those CMAQ results were available by 7:30 a.m. EDT. While results were not made available to the public in this first test season, they were made available to the participating scientists and to a focus group of potential customers for feedback. The extent of the modeling domain and example output for ozone are shown in Figure 3. Subsequent versions of the Eta-CMAQ forecast system will be expanded across the United States, and will add $PM_{2.5}$ forecast capability.

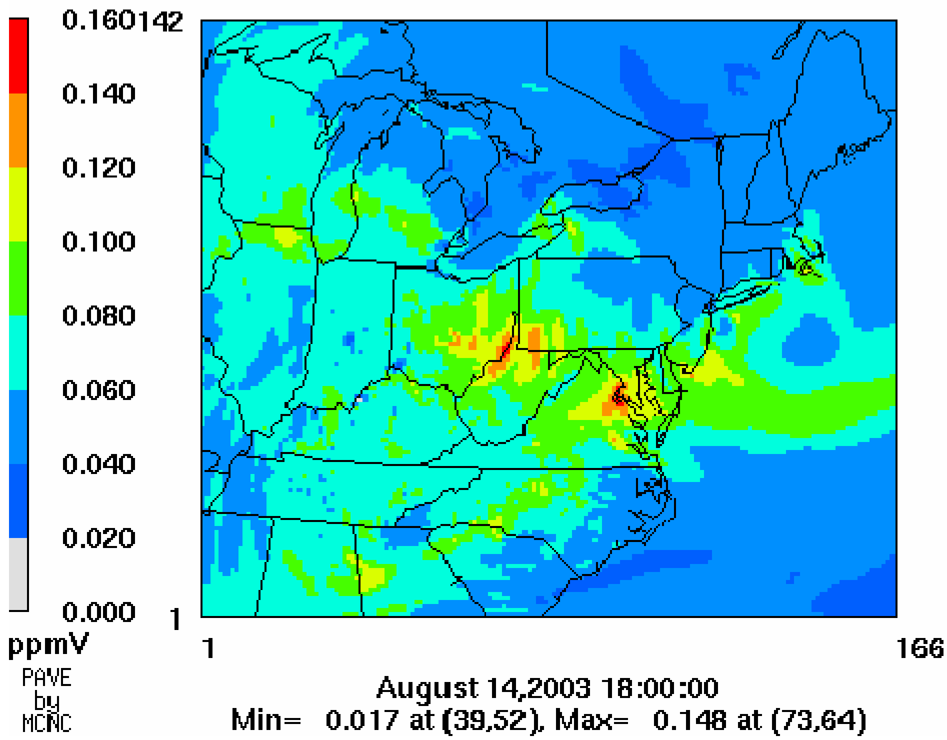

Figure 3. Ozone concentrations (ppm) at 2 p.m. EDT from the CMAQ air quality forecast model.

2.1.14 Linking Eta (Meteorological Model) with CMAQ for Air Quality Forecasting

As part of the development of the national air quality forecasting (AQF) system, a new software program was required to couple NCEP's Eta model with CMAQ. Before developing the software program, there were several practical and technical differences between the Eta model and CMAQ that needed to be considered. First, the Eta model uses a horizontal grid (Arakawa-E staggering), a vertical coordinate (step-wise terrain-following "Eta"), and a projection (rotated latitude-longitude) that CMAQ was not designed to handle. A major decision was whether to undertake the challenge of modifying CMAQ to adapt to the native grid systems used by the Eta model, or to interpolate Eta model output to a *familiar* grid structure and projection and potentially jeopardize the mass conservation in CMAQ. Ultimately, the Eta interpolation was selected for the AQF system. In addition, since CMAQ was run mostly with retrospective meteorological data, it was unclear whether or not the forecast output from Eta would contribute to reasonable ozone forecasts in CMAQ. Further, the Eta model creates a different suite of meteorological variables often using different internal physics modules than MM5, which had been coupled with CMAQ previously, so linking Eta and CMAQ required considering ways to best use the Eta output.

To enable a linkage between Eta and CMAQ, NCEP made several changes to the operational Eta system. For the AQF system, NCEP made hourly output files available (as opposed to the three-hourly files that are typically generated for external customers). In addition, NCEP added functionality to the Eta post-processor to vertically interpolate the Eta model output from the 60 step-wise vertical (Eta) layers to 22 hydrostatic sigma-P vertical layers that are compatible with the CMAQ system. NCEP added several output variables to the processing stream for use in AQF (*e.g*., PBL height, canopy conductance, plant canopy water). Finally, NCEP added new horizontal grids for the post-processed Eta model output that are specifically designated for the AQF system.

A key ingredient in the Eta-CMAQ linkage is a new pre-processor for CMAQ (PREMAQ) that was developed by ASMD and is largely equivalent to MCIP in the CMAQ model system. PREMAQ places the post-processed Eta model output into the required horizontal and vertical grids for CMAQ. Like MCIP, PREMAQ computes state variables and other derived variables (*e.g*., air density, Jacobian, dry deposition velocities for chemical species) that are required by CMAQ. Unlike MCIP, PREMAQ also includes calculations of the meteorologically dependent emissions (*i.e*., biogenic and mobile sources) adapted from SMOKE©. The output from PREMAQ includes the full set of meteorology and emissions files that are used by CMAQ.

There are several key differences between PREMAQ and MCIP. Of primary importance for NCEP is that PREMAQ processes the World Meteorological Organization standard GRIdded Binary (GRIB) files, which contain the data format used at NCEP and, by design, are unstaggered two-dimensional fields. PREMAQ also provides a full suite of grid geometry calculations (*i.e*., latitude, longitude, map-scale factors) from grid definition information in the GRIB headers. There are several modifications in PREMAQ to account for the different output variables generated by Eta compared to MM5. Notably, a new dry deposition routine, EtaDry, was developed for PREMAQ to take advantage of the land-surface fields that are output by the Eta model.

2.1.15 Preliminary Evaluation of Eta-CMAQ Forecast Model System

An operational evaluation of the coupled Eta-CMAQ forecast modeling system was performed in which both *discrete type forecasts* (observed versus modeled concentrations) and *categorical type forecasts* (observed versus modeled exceedances/non-exceedances) for both the maximum 1-hour O_3 concentrations (125 ppb) and 8-hour O_3 concentrations (85 ppb) were evaluated. The evaluation encompassed approximately three months (7 July–30 September 2003) and used hourly O_3 concentration data obtained from the EPA AIRNow network. Overall, the modeling system performed reasonably well in its first attempt at forecasting ozone concentrations. Results from the discrete evaluation revealed that correlations ranged from 0.59 (max. 1-hour) to 0.62 (max. 8-hour), normalized mean biases (nmb) ranged from 28.2% (max. 1-hour) to 37.3% (max. 8-hour), and the normalized mean errors (nme) ranged from 32.2% (max. 1-hour) to 39.9% (max. 8-hour). Results from the categorical evaluation revealed accuracy levels (which indicate the percent of forecasts that correctly predict an exceedance or non-exceedance) of 99.6% and 89.6% for the max. 1-hour. and max. 8-hour, respectively. Care must be taken in interpretation of this metric, however, as it is greatly influenced by the overwhelming number of non-exceedances. To circumvent this inflation, another metric called the *Probability of Detection* was calculated. This metric ranged from 16.7% (max. 1-hour) to 41.0% (max. 8-hour), and measured the number of times a model predicted an exceedance when one actually occurred.

An error was discovered midway through the forecast period in Eta's post-processed land-use designation that resulted in the underestimation of dry deposition, and, hence, led to the overestimation of ambient concentrations. To investigate the significance of the error, an 8-day period (12–19 August) was re-simulated and re-evaluated. With the correction, the nmb fell from 27.5% to 13.0% for max. 1-hour and from 37.2% to 20.1% for max. 8-hour. The nme were also significantly reduced, falling from 31.7% to 21.7% for max. 1-hour and from 39.9% to 26.3% for max. 8-hour. The correlations between observation and modeled ozone values also increased for both the max. 1-hour and max. 8-hour. The short duration and dearth of exceedances precluded calculation of categorical evaluation metrics for the corrected simulation.

2.2 Atmospheric Model Evaluation and Application Activities

2.2.1 Developing a Strategy for Assessing Performance of Regional-Scale Air Quality Models

Developing model performance metrics for regional-scale air quality models is a work in progress. There are many sources of uncertainty, including boundary conditions, emissions, chemistry, and transport. Complications arise because regional-scale models provide volume-average concentrations, whereas the observations are daily averages on a one-in-three day sampling interval at specific sparsely-spaced points. During 2003, investigations were conducted of 1) regional-scale modeling to gain an understanding of whether the available monitoring data is suitable to assess an increase in the model skill if smaller grid sizes are used, and 2) monitoring data to gain an understanding of the extent observations collected by different monitoring networks can be combined.

In the first investigation, Gego *et al.*, (accepted for publication)(a) examined temperature and ozone observations and model predictions for three high ozone episodes that occurred over the northeastern United States during the summer of 1995. In the first set of simulations, the meteorological model RAMS4a was run with three two-way nested grids of 108-, 36-, 12-km grid spacing covering the United States and the photochemical model UAM-V was run with two grids of 36-, 12-km grid spacing covering the eastern United States. In the second set of simulations, RAMS4a was run with four two-way nested grids of 108-, 36-, 12-, 4-km grid spacing and UAM-V was run with three grids of 36-, 12-, 4-km grid spacing with the finest resolution covering the northeastern United States. The analysis focused on the comparison of model predictions for the finest grid domain of the simulations, namely, the region overlapping the 12 km and 4 km domains. Comparisons of 12-km versus 4-km temperature and ozone fields showed that the increased grid resolution leads to greater texture in the model predictions; however, comparisons of model predictions with observations did not reveal the expected improvement in the predictions. Hence, while high-resolution modeling has scientific merit and potential uses, it is uncertain how one would assess the accuracy of the high-resolution model predictions with the currently available monitoring networks.

In the second investigation, Gego *et al.*, (accepted for publication)(b) examined airborne fine particulate matter in the United States as monitored by three different networks: the Clean Air Status and Trend Network (CASTNet), the Interagency Monitoring of PROtected Visual Environment Network (IMPROVE), and the Speciation and Trend Network (STN). If combined, these three networks provide speciated fine particulate data at several hundred locations throughout the United States. Differences in sampling protocols and samples handling might preclude their joint use. With these concerns in mind, the objective of this study was to assess the spatial and temporal comparability of the sulfate, nitrate, and ammonium concentrations reported by each of these networks. One of the major differences between the networks is the sampling frequency they adopted. While CASTNet measures pollution levels on 7-day integrated samples, STN and IMPROVE data pertain to 24-hour samples collected every three days. STN and IMPROVE data, therefore, exhibit much more short-term variability than their CASTNet counterpart. Despite their apparent incongruity, averaging the data with a window size of four weeks was sufficient to remove the effects of differences in sampling frequency and duration and allow meaningful comparison of the sulfate and ammonium concentration values reported by the three networks. After averaging, all the sulfate and, to a lesser measure, ammonium concentrations reported by the three networks are fairly similar. Nitrate concentrations, on the other hand, were still divergent. It was speculated that this divergence originates from the different types of filters used to collect particulate nitrate. Finally, rotated principal component analysis (RPCA) was used to determine if there were subregions where the temporal modes of variation detected by each network were similar for the three pollutants of interest. For sulfate and ammonium, the subregion boundaries established for each network and the modes of variations within each cluster seemed to correspond. For the CASTNet and IMPROVE networks, RPCA performed on nitrate concentrations revealed that the modes of variation did not correspond to unified geographical regions but were found more sporadically. For STN, the clustered areas were unified and easily definable. Hence, the possibility of jointly using the data collected by CASTNet, IMPROVE, and STN has to be weighed pollutant by pollutant. While sulfate and ammonium data show some potential for joint use when averaged over a 4-week window at this point, combining the nitrate data may not be a judicious choice.

The results of these two investigations provide clues of how to conduct a first-order evaluation of regional-scale model performance. The first investigation suggests the available monitoring data and modeling results are best suited to assessing long-term variations in time and larger spatial domain. The second investigation suggest there are local contiguous subregions where monitoring results may have similar temporal behavior. These results suggest the following strategy for assessing model performance. From a principle component analysis the subregions in the monitoring data can be identified. Following the application of a 5-week running average to the observed and modeled values, an assessment of the performance of the regional-scale model can be conducted in each subregion. Assessing regional-scale model performance on their ability to characterize the long-term seasonal time series in this manner is seen to provide a first-order means for detecting gross sources of bias and would provide a basis for a first-order quantitative comparison of the relative performance of several models.

2.2.2 Developing and Testing an ASTM Strategy for Assessing Performance of Local-Scale Dispersion Models

During the development phase of an air quality dispersion model and in subsequent upgrades, model performance is constantly evaluated. These evaluations generally compare simulation results using simple methods that do not account for models only predicting a portioning of the variability seen in the observations. To fill a part of this void, a standard was developed and adopted by the American Society for Testing and Materials (ASTM, 2000), designation *D6589 Standard Guide for the Statistical Evaluation of Atmospheric Dispersion Model Performance*. In the annex to this standard is an example method that tests the ability of dispersion models to simulate the average centerline concentration. The method involves grouping observed data into groups or regimes, in which the dispersion is expected to be somewhat similar. The average centerline concentration is then derived for each group using bootstrap resampling. It is this average centerline concentration that is then compared with the modeling results. By this means, the focus is on testing the ability of models to replicate the first moment, the average, of the centerline concentration distribution, which for most operational models is the only feature in the centerline concentration distribution they are capable of simulating. Recent work (Irwin *et al.*, 2003) was conducted to further test the ASTM example test method. This work involved the application of the test method to the results from ADMS version 3.1, AERMOD versions 98022 and 02161, HPDM version 4.3, level 920605, and ISCST3 version 00101. Three atmospheric dispersion field studies are analyzed: Prairie Grass 1956 rural, low level release (Barad, 1958; Haugen,1959); Kincaid 1980 rural, elevated release (Bowne *et al.*, 1983); and Indianapolis 1985 urban, elevated release (Murray and Bowne, 1988). Following the ASTM method, the normalized mean square error (NMSE) was used in comparing the performance of the five models over the three field experiments. The base models, those having the lowest value of NMSE, were seen to be AERMOD version 02161 for Prairie Grass, and HPDM for Kincaid and Indianapolis. Even though NMSE for ADMS was larger than that for AERMOD, it was noticed that for Kincaid the results for AERMOD were found to be significantly different from that found for HPDM the base model. This occurred because the bootstrap-derived standard deviation of the NMSE for the ADMS results was sufficiently large to encompass the HPMD results, whereas the bootstrap-derived standard deviation of the NMSE for the AERMOD results did not encompass the HPDM results. This result suggests there may be inappropriately grouped data for some of the analyses, and that future investigations should conduct a detailed investigation into each group to insure that questionable observations are not unduly influencing the results. An underlying assumption in grouping data together is that they will provide a representative average centerline concentration value. If the data are poorly grouped, then the average centerline concentration for the regime would likely be biased too low, concerns of which were expressed by Olesen (2001).

2.2.3 Inverse Modeling for Ammonia

One of the key uncertainties affecting air quality model predictions is the uncertainty in the emissions input. Ammonia emissions have one of the highest degrees of uncertainty compared to other emissions, and they have an impact on fine particle predictions. Variations in ammonia emissions will cause large variations in predicted nitrate PM concentrations. The EPA National Emission Inventory (NEI) for ammonia emissions is based on a 1994 report, which extrapolated European emission factors for the United States. These emission estimates suggest that the largest source of ammonia emissions is animal husbandry, which comprises about 80 percent of the total. Fertilizer is also a substantial source. Both of these sources are expected to have seasonal variations because of the temperature dependence of ammonia volatilization from animal waste and because of the seasonal patterns in fertilizer application. However, the emission factors used in the NEI do not have any dependence on temperature, and great uncertainty exists in the factors themselves. For these reasons, the uncertainty in ammonia emissions is due to their seasonality and in their overall annual magnitude.

Ammonia emission studies traditionally were based on flux observations at individual sites, which are dependent on such local factors as the meteorological conditions, housing conditions, and feed for the animals studied. To evaluate the current ammonia emissions inventory on a regional scale, inverse modeling is used to estimate monthly ammonia emission fields for the eastern United States. Using a Kalman Filter-based technique with CMAQ, inverse modeling is used to estimate monthly ammonia emissions that produce optimized predictions of wet concentrations of ammonium for 1990. Further, uncertainties in the modeled precipitation were accounted for by introducing the standard error of the precipitation estimate into the Kalman filter. Results suggest that the emissions should be highest during summer conditions and lower during fall and winter (Gilliland *et al.*, 2003).

As a next phase of this study, inverse modeling tests for ammonia will be extended to the United States continental domain where an annual simulation is already planned for CMAQ model evaluation. The work will also be extended to examine such different sources of emissions as cattle and hogs. The objective is to assess whether a particular source has a greater degree of uncertainty than other sources and to consider spatial uncertainty in the emissions based on source-specific information. The ammonia emission estimates developed from this study support the work of OAQPS, which is currently evaluating the NEI ammonia inventory and developing an updated ammonia inventory based on newer research. This work also supports the air quality modeling community whose modeling results can be detrimentally affected by large uncertainties in ammonia emission inputs to the model.

2.2.4 Diagnostic Metrics for Ozone and Particulate Matter

Diagnostic metrics enable us to examine the process side of the model to better study the degree of reliability of control strategy predictions. They require a special set of non-routine measurements, because they typically involve ratios of species involved in photochemical production. Earlier work (Tonnesen and Dennis, 2000a; 2000b) had identified a set of metrics based on measurement of O_3, NO+true NO_2 = NO_X, NO_Y, and NO_Y-NO_X = NO_Z. These diagnostic tests were applied to CMAQ for Nashville, Tennessee, for the 1995 SOS field measurements (Arnold *et al*., 2003). The model simulations examined for Nashville with 12-km and 4-km horizontal grid cell sizes. The modeling results from 36-km grid spacing were not examined because they were considered to be too coarse for ozone predictions for a moderate-sized urban area. The diagnostic metrics suggest that the 4-km grid cell size produces slightly better predictions relative to ozone process fidelity. Current work is examining differences among the three chemical mechanisms in CMAQ with the help of sensitivity analyses that include emission reductions. The metrics also highlighted sites that were being influenced by local emission sources missing in the model, pointing out sites where model prediction of ozone changes might be biased because of missing emissions (or extra emissions) in the model inputs. New statistical test procedures for the quantitative comparison of ozone production efficiencies, including uncertainty limits, are being developed as part of this work because the metric used to define ozone production efficiency, the relationship between hourly O_3 and aged nitrogen oxides (NO_Z), as typically illuminated in scatterplots, is curvilinear and involves effectively two independent variables, rather than dependent and independent variables. Thus, standard procedures are not appropriate. Also, approaches for quantitative comparison of data partitioned into bins will be developed next year. The metrics are now being applied to other time periods, SOS Nashville 1999 data, and other cities, SOS Atlanta 1999, and South East Aerosol Research and Characterization 1999, to test their robustness.

2.2.5 CMAQ Model Evaluation to Assess Readiness for State Implementation Plans

The 2003 release of CMAQ was made available during August. As part of this release, an operational evaluation was performed involving two simulation periods (January 4–February 19, 2002, and June 15–July 16, 1999), using two chemical mechanisms, SAPRC and CB-IV. Only the SPARC simulations are presented here. Full evaluation results from the other simulations as well as release notes documenting model changes and updates are available at www.epa.gov/asmdnerl/models3/index.html. The summer simulation was performed using a 32-km resolution over the entire United States domain with a vertical resolution of 21 layers set on a sigma coordinate; while the winter simulation used a 36-km grid resolution and 24 vertical layers. For both simulations, the meteorological fields were derived by MM5 and were processed through MCIPv2.2. Emissions of gas-phase SO_2, CO, NO, NO_2, NH_3, and VOCs were based on the 1999 EPA NEI. Primary anthropogenic $PM_{2.5}$ emissions were separated into different species, including particle SO_4, NO_3, OC, EC. Emissions of HC, CO, NO_x, and PM from cars, trucks, and motorcycles are based on Mobile5b, while biogenic emissions were obtained from BEIS3.12.

Operational data used in the evaluation were obtained from four nationwide networks. Hourly O_3 (ppb) data were obtained from over 700, mostly urban, Aerometric Information Retrieval System (AIRS) stations over the 4-week summer evaluation period. Weekly average concentrations of SO_4^{2-}, NO_3^-, HNO_3 and NH_4^+ ($\mu g\ m^{-3}$) were obtained from nearly 70, mostly rural CASTNet stations. Four weekly collection periods coincided with the summer simulation period; while six were available for the winter simulation. Daily average concentrations of SO_4^{2-}, NO_3^-, $PM_{2.5}$, OC, and EC ($\mu g\ m^{-3}$) from 50 rural IMPROVE sites were also used. These data are collected on every third day, (midnight to midnight, local time), limiting the number of days available for comparison to 10 and 15 for the summer and winter simulations, respectively. Finally, data from the more recently established STN, which follows the protocol of the IMPROVE network (*i.e.*, every third day collection) were obtained from 60, mostly urban sites. The STN provided measurements of SO_4^{2-}, NO_3^-, $PM_{2.5}$, NH_4^+, OC and EC ($\mu g\ m^{-3}$) for 15 days during the winter simulation.

Examination of the tables reveals that CMAQ produces fairly unbiased Normalized Mean Biases (NMB) <10%, and accurate Normalized Mean Errors (NME) ~ 20.0% simulations of both the max.-1 hour and max.-8 hour ozone concentrations when compared against the AIRS data. Correlations are also fairly good (between 0.72 and 0.75) indicating that CMAQ is capturing roughly 50% of the variability exhibited by the observations. CMAQ performs quite well in simulating SO_4 concentrations. Correlations are high, ranging from 0.90 during the summer against both CASTNet and IMPROVE sites to 0.66 in the winter against STN sites. The NMBs are, with one exception, positive and between 9.2 and 38.4%. The lone underprediction occurs against STN data, NMB: -12.0%, and like the lower correlation, may be attributable to the urban nature of the STN. The NMEs range from 25.7% (winter, CASTNet) to 61.9% (summer, IMPROVE). Of all of the species simulated by CMAQ, NO_3 simulations are the worst. Correlations are lower for the winter simulations (0.27: CASTNet, 0.36: IMPROVE) when compared to the summer simulations (0.39: STN, 0.54: IMPROVE, 0.76 (CASTNet). The summer simulation produces negative biases (NMB: -30.8% for CASTNet, -39.1 for IMPROVE), while NMBs for the winter simulation are mixed, ranging from 8.0% for STN to 46.8% for CASTNet. The errors associated with NO_3 simulations are generally the largest produced by CMAQ and range from 66.9% (winter, STN) to 96.5% (winter, IMPROVE).

Results of NH_4 simulations mirror those of SO_4 in that CMAQ performs quite well and consistently, especially when compared against CASTNet observations (correlations: 0.86 summer simulation, 0.85 winter). As seen with SO_4 and probably for the same reason, the CMAQ correlation against the STN is considerably lower (0.41). The NMB against STN data is however small (5.2% for the winter simulation) when compared against CASTNet (40.0% for the winter and 22.7% summer). The NMEs range from 36.5% (summer CASTNet) to 57.7% (winter STN). The results of the $PM_{2.5}$ simulations are like $PM_{2.5}$ itself, a composite of the other species.

Correlations associated with the more rural IMPROVE network are considerably higher (0.71 summer, 0.68 winter) than those associated with the more urban STN network (0.37 winter). The NMB for the summer simulation is small and negative (-9.8%) against the IMPROVE network, small but positive for the winter simulation against STN and large and positive for the winter simulation against the IMPROVE network. The NME range from 40.3% (summer simulation against IMPROVE) to 57.7% (winter simulation against STN).

The results associated with the HNO_3 evaluation are consistent between the summer and winter simulations. The correlation for the summer simulation is 0.79, while that for the winter is 0.64. The NMBs are positive (49.0, 44.2 for summer, winter respectively) and the NMEs average near 60%. Results for OC are mixed depending on season and network. The NMB against IMPROVE is small and negative (-1.5%) in the summer yet it is positive and larger in the winter (17.2%). Against the STN data, the winter CMAQ simulation significantly underpredicts (NMB: -50.0%). The NMEs are more consistent, though large, ranging from 60.4% to 70.0%, and the correlations ranging between 0.32 and 0.56. The summer CMAQ simulation of EC is unbiased (NMB: 1.0%) and produces a correlation of 0.69 when compared against IMPROVE data. Conversely, the winter simulation significantly overpredicts EC, resulting in large positive biases (31.0% and 59.1% against IMPROVE and STN respectively) and large errors as well (NME 81.0%, and 95.0%).

Table 1. Summer 1999 evaluation statistics

Species	O_3 (Max-1)	O_3 (Max-8)	SO_4		NO_3		$PM_{2.5}$	NH_4	HNO_3	OC	EC
Network	AIRS	AIRS	CAS	IMP	CAS	IMP	IMP	CAS	CAS	IMP	IMP
n	23,196	23,196	264	490	264	415	457	264	264	396	396
r	0.72	0.75	0.90	0.90	0.27	0.36	0.71	0.86	0.79	0.32	0.69
MB	2.3	4.3	1.74	0.75	-0.15	-0.11	-0.73	0.31	1.11	-0.02	0.00
NMB (%)	3.8	8.7	38.0	38.4	-30.8	-39.1	-9.8	22.7	49.0	-1.5	1.00
RMSE	14.5	12.8	2.89	2.37	0.57	0.51	4.70	0.70	1.77	1.35	0.24
NME (%)	18.8	20.2	46.4	61.9	75.7	95.0	40.3	36.5	58.7	67.2	52.6

Table 2. Winter 2002 evaluation statistics

Species	SO_4			NO_3			$PM_{2.5}$		NH_4		HNO_3	OC		EC	
Network	CAS	STN	IMP	CAS	STN	IMP	STN	IMP	CAS	STN	CAS	IMP	STN	IMP	STN
n	407	1149	728	407	1044	688	927	714	407	1149	407	731	1106	731	1148
r	0.83	0.66	0.85	0.76	0.39	0.54	0.37	0.68	0.85	0.41	0.64	0.56	0.47	0.55	0.40
MB	0.15	-0.26	0.29	0.64	-0.27	0.20	0.51	1.49	0.33	0.07	0.55	0.14	-1.64	0.07	0.42
NMB (%)	9.2	-12.0	31.5	46.8	-8.0	28.9	4.1	40.3	40.0	5.2	44.2	17.2	-50.0	31.0	59.1
RMSE	0.60	1.16	0.72	1.36	4.37	1.26	10.45	3.81	0.51	1.46	1.07	0.93	3.32	0.48	1.17
NME (%)	25.7	35.9	53.1	70.4	66.9	96.5	50.0	68.9	47.2	57.7	61.3	70.0	60.4	81.0	95.0

2.2.6 Sensitivity of CMAQ Control Strategy Predictions to Model Input Uncertainties for CMAQ and MM5 Configurations

Sensitivity analyses are important adjuncts to model-data comparisons. A key use of the air quality models is prediction of the effects of emission controls on air concentrations. Air quality models are used in the State Implementation Plan (SIP) process to assess impacts of potential emissions reduction strategies for the criteria pollutants, in particular ozone. These predictions can be affected by model input uncertainties, model parameter uncertainties, and structure of the model itself. One area of concern is the choice of vertical mixing algorithms because they alter the species concentration mixing histories and, hence, the photochemical processing, potentially altering the control strategy response from CMAQ. Two choices were targeted for the sensitivity analysis because the first represents new science, ACM, offered within CMAQ choices, and the second represents an important change made by the CMAQ developers to the default configuration of the vertical eddy diffusivity option (K_Z) in CMAQ to account for severe nighttime overprediction of conservative species. The results were:

Change in base year O_3 simulation. The physics sensitivities had a noticeable effect on the simulation of the base year ozone. For the ACM version at the nonurban sites, the change in daytime O_3 spanned 40-45 percentage points and was predominately an increase, from a -5% change to a +35% change. For the old K_Z version, the change in daytime O_3 spanned 30-40 percentage points with larger increases than decreases, from a -10% change to a +20% change. At the large urban site for both sensitivity versions the changes were more evenly divided between negative and positive, spanning from a -30% to a +40% change in daytime O_3.

Change in control strategy response. The physics sensitivities had only a small effect on the simulation of the relative response of O_3 to a precursor emission reduction. The majority of the differences in the predicted percent relative reduction factors were less than +/-0.5 percentage points and most of the rest of the differences less than +/-1%. In contrast, the control strategy response for the NO_x emission reductions ranged from a 30% decrease to a 10% increase, and up to a 130% increase for a few daytime hours for the large urban area. The control strategy response for the VOC emission reductions ranged from zero to a 17% to 20% decrease.

Insignificant dependence on grid size. The dependence of the sensitivity response on grid size for either the base year response or the control strategy response was very small.

Correlation between base simulation change and control strategy simulation change. The base year O_3 changes due to the sensitivity were not at all correlated with the differences in the relative control strategy response caused by the sensitivity.

An important observation is that the base year O_3 changes in sensitivity is not to be correlated with the differences in the relative control strategy response caused by the sensitivity. Sensitivity analyses investigate uncertainties by directly evaluating the effect of the uncertainty on the control strategy prediction. Based on this analysis, a recommendation for CMAQ users is that they stay close to the CMAQ default value and not be unduly influenced or concerned by the nighttime performance for O_3 in base year simulations. A paper on this sensitivity analysis is being prepared.

The sensitivity analysis is being extended to the chemical mechanism choices in CMAQ as a chemistry sensitivity. Based on completed chemical mechanism sensitivity runs, preliminary analyses suggest that while differences in the type of vertical mixing (physics parameterizations) used create comparatively much larger differences in predicted daily ozone for the base simulation period, differences in chemical mechanisms, however, systematic differences among different chemical mechanisms are seen in regard to the control strategy response.

2.2.7 Model Evaluation Toolkit

ASMD initiated the development of a prototype model evaluation toolkit. The intent of the toolkit is to provide specialized data analysis capabilities for supporting the comparison of model results with observations. For instance, Murphy *et al*. (1989) and Taylor (2001) describe specialized data plots that provide better insight into how well a model's results corresponded with observations than the types of plots that are typically available. The prototype toolkit has been implemented in R, an open source statistical package. Users can easily combine R's powerful data manipulation and statistical capabilities with the model evaluation toolkit's features. The toolkit was designed to be used in a variety of applications. It provides general data structures for gridded and point data, methods for converting between the data structures, temporal averaging functions, standard performance measures, and specialized plots.

2.2.8 Meteorological Model Evaluation

Air quality modeling simulations are strongly dependent on the meteorology. Thus, the performance of meteorological simulations must be assessed in conjunction with the chemical-transport predictions. Traditional verification methods do not take advantage of the increasing amounts of non-standard meteorological observations (*e.g*., wind profilers, aircraft, satellite winds, etc.). During FY-2003, initial development was completed on a meteorological evaluation system, which provides an efficient method to comprehensively assess modeled meteorology using both traditional and non-standard observations. The core of the evaluation system is automated to allow efficient evaluation of lengthy simulations.

The backbone of the model evaluation tool is flexibility, allowing more than one type of model and many types of observations to be evaluated. Models that were tested include the PSU/NCAR MM5, NCEP Eta model, and the WRF model. Additionally, many types of observational data sets are compatible with the system. The core of the evaluation section of the system currently consists of plug-in modules that compute traditional model statistics on surface observations, temperature, moisture, wind, precipitation, and radiation, using specific criteria.

Newer sophisticated techniques are planned for development. For example, one of these techniques will use wind profiler data to estimate boundary-layer depth for comparison with model values. Other techniques will take advantage of averaging and filtering of data to examine whether or not temporal and spatial variability is properly represented. Several model data sets have facilitated the development and testing of the model evaluation tool in FY-2003.

2.2.9 Sub-Canopy Deposition Models

Biologists and plant physiologists interested in studying the effects of pollutants on vegetation have learned that it is not sufficient to relate plant symptoms to local pollutant concentration. The concentration of pollutants in the air above or near the plant canopy is not the same as the amount of pollutants that actually gets into the plant, or its exposure, which for the same concentration can vary depending on species, weather, time of day, season of the year, and health of the plant. While models do a good job of predicting exposure of the total canopy, normal deposition models are not designed to operate within the canopy at the leaf level, where pollutant damage occurs. Yet, understanding deposition at the leaf level is necessary to access the plant-damage relationship. To estimate dosage and exposure, a model designed to estimate fluxes and plant exposure within a plant canopy is needed. However, a sub-canopy model is not simple. Because wind and pollutant profiles within a canopy are not log-linear as they are in the normal atmospheric boundary layer, simple gradient-transfer models are inappropriate. Higher-order closure models have been developed for this purpose. These models were developed for use in tree canopies, but have received little evaluation. For use in herbaceous perennials, which are frequently studied because of their sensitivity to pollutants, these models were not evaluated. ASMD has started a model evaluation and improvement program for this reason, adapting a higher-order closure model developed by NOAA's Atmospheric Turbulence and Diffusion Division (ATDD) at Oak Ridge, Tennessee, and collaborating with ATDD in the evaluation and improvement program. This study is part of a larger study of ozone damage to sensitive plants, with additional collaborators at Auburn University, Auburn, Alabama, University of Newcastle, United Kingdom, and Appalachian State University, Boone, North Carolina.

A preliminary field study was completed in the summer of 2002 at Purchase Knob in the Great Smoky Mountains National Park, a high elevation location set aside by the National Park Service for educational and scientific activities. Two study sites were selected, one on the outside edge of a forest, and one inside the forest where the plants grew in dappled shade. The species under study was cutleaf coneflower (*Rudbeckia laciniata*), which has been shown to be very sensitive to ozone. Populations of this plant are not uncommon in the park at higher elevations.

Selected results from the 2002 study are shown below. Figure 4 displays measured and modeled ozone concentrations at three levels in a stand of coneflowers that was growing under the forest canopy. The model reproduced the observed values very well in the middle of the canopy at 0.78 m, but overpredicted the ozone at the lower height near the ground. Figure 5 compares the predicted and observed turbulent energy above the canopy at 1.5 m. The model overpredicted vertical (w'^2) turbulent energy, but underpredicted the horizontal turbulent energy. The observed values of u'^2 and v'^2 are similar. This is not typical of a normal boundary layer, and may be a result of the redistribution of energy by the tree trunks.

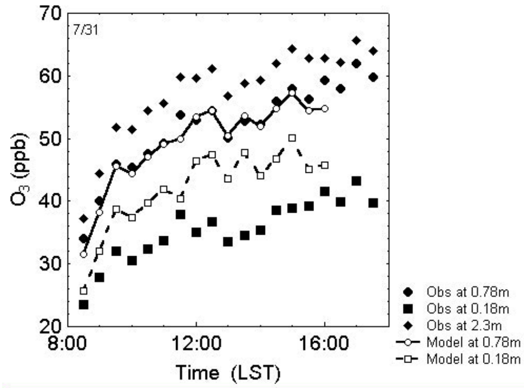

Figure 4. Observed and modeled ozone.

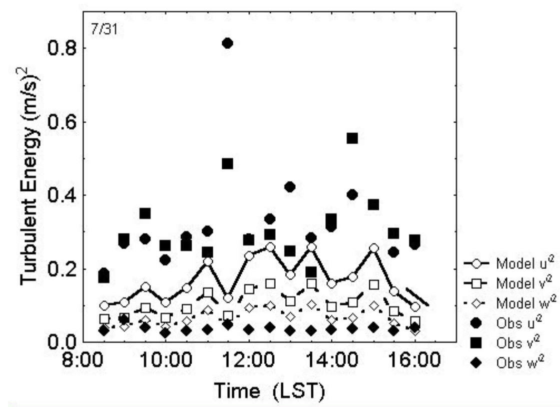

Figure 5. Observed and modeled variance of the wind speed

In August of 2003, a second field study was conducted to gather a more complete data set for sub-canopy model evaluation. The study was conducted in the same location as the 2002 study, at Purchase Knob in the Great Smoky Mountains National Park (Figure 6). Some differences between the 2002 preliminary study and the 2003 study were: (1) the study ran for three weeks, instead of four days, and much more data were gathered, (2) a second sonic anemometer was employed to measure turbulence within the plant canopy (Figure 7), and (3) a new ozone profile measurement system was built, which used only one ozone monitor, sampling different levels sequentially. This approach avoided bias between multiple ozone monitors sampling at the same time. Figure 8 shows the sampler, and Figure 9 the sampling tubes and filters located in the coneflower canopy. Finally, (4) the height and leaf area index (LAI) of the coneflower stand were measured every two weeks from the emergence of the plants in May until maturity in late August. This data will be used to model the total growing season exposure of the plants, and relate it to observed plant injury.

The 2003 Purchase Knob field study resulted in an extensive data set of ozone profiles, wind and turbulence measurements, and plant physiological data. The data are being analyzed and will be used to evaluate the NOAA-ATDD sub-canopy deposition models. Also, the data will be used with Lagrangian near-field dispersion analysis to help understand the nature of the ozone sinks in the sub-canopy environment.

Figure 6. Study location at forest edge behind the NC air monitoring station.

Figure 7. Sonic anemometer in canopy.

Figure 8. Ozone profile sampler.

Figure 9. Profile sampling tubes.

2.2.10 Modeling Studies in the Mid-Atlantic Region

Simulations with the Extended RADM were used in a joint effort with the National Park Service to develop an environmental assessment for the SHENandoah National Park (SHEN). The SHEN assessment report was released in August 2003 (Sullivan *et al*., 2003). Such an assessment is unique in National Park Service history in that its Natural Resource Protection Program funds were allocated to a state-of-the-science assessment for a national park. This was in part due to the documented loss of a fish species in the SHEN during the 1990's, indicating the current reductions in sulfur and nitrogen deposition are inadequate.

The SHEN Assessment addresses air quality related values (AQRV's) and key air pollutants that threaten aquatic resources primarily from sulfur and nitrogen deposition, terrestrial resources primarily from O_3 exposure and nitrogen and sulfur deposition, and visibility primarily from sulfate fine particles. The Extended RADM was used to create regional air quality analyses and characterize the sources of air pollution affecting SHEN for 1990 emission conditions and to estimate changes at the park in sulfur and nitrogen deposition and sulfate and ozone air concentrations stemming from potential future reductions in SO_2 and NO_x emissions. To assess current contributions, airsheds were developed to indicate the principal source regions responsible for the majority of acidic deposition and sulfate haze affecting the park. Also, the relative contribution of airshed states to the acidic deposition and sulfate haze were defined and the top-ranked source hot spots contributing to air pollution were identified. To estimate future conditions, emission projections developed by the EPA Clean Air Markets Division and combined with heavy duty diesel rule projections from EPA's OAQPS were simulated with the Extended RADM. Relative changes from the Extended RADM were provided to ecological models for calculations of 1990 to 2020 changes to visibility and aquatic and forest resources. The assessment reveals that the park's visibility and sensitive aquatic ecosystems have been significantly impaired by human-caused air pollution, and that sensitive resource recovery would fall substantially short of necessary improvements unless very aggressive emission reductions occur, reductions well beyond Clean Air Act regulations as of mid-2003. The SHEN assessment is posted at the web site for the National Park Service Air Resources Division (www2.nature.nps.gov/ard).

2.2.11 Bay Regional Atmospheric Chemistry Experiment: Model Evaluation

The Tampa Bay Estuary Program and the Florida Department of Environment (FDEP) have asked the EPA/National Exposure Research Laboratory (NERL) and NOAA/Air Resources Laboratory (ARL) to enter into a partnership to apply CMAQ to understand the sources of nitrogen deposition affecting Tampa Bay. The majority (60 percent) of the nitrogen deposition to the estuary and watershed is estimated to come from sources local to Tampa Bay, which is unusually high, due to Tampa's isolation from other large source regions. ASMD was asked to work with the Tampa Bay National Estuary Program to assess the atmospheric contribution of nitrogen to Tampa Bay. Tampa Bay provides an important atmospheric multimedia problem involving coarse particles and sea salt. Two of the largest power plants in the nation, in terms of

NO_x emissions, are on the shores of the Bay and there are serious questions as to how much of the atmospheric deposition is due to the power plants versus mobile sources in the area surrounding the Bay. CMAQ was selected as the model for the Tampa Bay Assessment, in part because CMAQ will incorporate sea salt in its fine particle module in FY-2003. Prior to any Tampa Bay assessment, it was agreed that CMAQ needs to be evaluated against high-quality local data and that the nitrogen budget around Tampa Bay needs to be more carefully characterized.

The Bay Regional Air Chemistry Experiment (BRACE), designed for the above two purposes, was conducted during May 2002. Division scientists, along with ARL colleagues, were involved in the planning of BRACE. Division scientists played a major role in establishing the location of the BRACE supersite and in establishing the suite of measurements for the supersite and several surrounding measurement sites that would to the best degree feasible delineate the full nitrogen budget and photochemical processing behind the budget. ASMD scientists worked on deployment of true-NO_2 monitors and with Hillsborough and Pinellas Counties' air quality professionals on deployment of NO_Y instruments. ASMD and NOAA ARL, Silver Spring, Maryland, scientists took the lead on siting three wind profilers around the Bay, and helped define the complete chemistry package of instruments for the NOAA Twin Otter aircraft flown by ARL.

The Wexler sectional aerosol model, Aerosol Inorganic Model (AIM), was adapted to incorporate sea salt in its calculations. During FY-2003, this sectional model was implemented into the 2002 release version of CMAQ. CMAQ-AIM was tested and successfully adapted to run on multiple Linux CPU's. The first calculations for the period of July 4–14, 1999, were completed and compared to the CMAQ 2002 version. Results are to be presented in the BRACE session at the Fall 2003 American Geophysical Union meeting. In early FY-2004, the Wexler AIM sectional aerosol module is to be incorporated into the September 2003 release version of CMAQ for a more current CMAQ-AIM version.

2.2.12 Recommendations for Observations-Based Methods **Sherry delete this title and whole section**

2.3 Air Toxics Modeling

2.3.1 National Air Toxics Assessment

The National Air Toxics Assessment (NATA) is designed to help EPA, state, local, and tribal governments and the public better understand the air toxics problem in the United States. The national-scale assessment includes four steps:

1. Compiling an inventory of air toxics emissions,
2. Estimating the annual average outdoor air toxics concentrations,
3. Estimating the exposure concentrations (what people are estimated to breathe), and
4. Characterizating of potential public health risks.

In general, larger urban areas appear to carry greater risk burdens than smaller urban and rural areas, because the air toxic emissions tend to be higher in areas with more people. This trend is not universal, and can vary from pollutant to pollutant, according to their sources. Additionally, NATA has not focused on the identification of geographic areas or populations that have significantly higher risks than others. Rather, it has focused on characterizing ranges of risks across the country independent of their location. The highest localized inhalation exposures and risks are not captured by this national-scale approach. It is important to use local-scale assessments to characterize exposures and risks very close to specific sources.

To address this issue, many regional and community scale modeling assessment projects are now underway. For the Philadelphia regional scale assessment, the Division is collaborating with EPA Region 3 to identify and correct problems in the emission inventory, which will be run in a local scale dispersion model utilizing the improved particulate and gaseous deposition algorithms recently implemented in the AERMOD dispersion model. Results will be used to refine plans for regional and local air toxic control efforts.

Although large uncertainties (*e.g.*, emission levels, exposure, toxicity) are inherent in this analysis, the modeling results can be interpreted in a relative rather than absolute manner. For example, the results are appropriate to answer such questions as which pollutants or source sectors may be associated with higher risks than others (*e.g.*, priority setting for data collection), but not for determining exactly how many people are exposed to certain levels of absolute risk (*e.g.*, to determine what's safe and what's not).

2.3.2 Fine-Scale Modeling of Air Toxics and Homeland Security

This effort seeks to develop and evaluate numerical and physical modeling tools for simulating ground-level concentrations of airborne substances in urban settings at spatial scales ranging from ~1-10 km. These tools will support modeling needs for air toxics and homeland security. The air toxics tools will benefit EPA's NATA program and contribute to the improvement of human exposure models. The homeland security-related portion of this task will help in developing tools to assess the threat posed by the release of airborne agents. Both sets of tools will consider the effects induced by urban morphology on fine-scale concentration distributions.

Due to source distributions and photochemical activity, airborne substances can exhibit different degrees of spatial and temporal variability, especially in urban areas and in different geographical-climatic regimes. Because current observation networks for driving exposure models are inadequate, human exposure assessments need to be driven by air quality simulations performed at the scale of census tracts. Exposure models need ambient concentration fields at neighborhood-scale resolution to address such issues as environmental justice, community-based risk assessments, and for conducting hot spot analyses. The Models-3/CMAQ modeling system is being applied with horizontal grid cell dimensions ranging from 36 km to 4 km to provide concentration distribution at regional to urban scales respectively. There is a need to improve the capability of current tools to perform model simulations that can provide accurate simulations at neighborhood scale resolutions. Homeland security modeling requirements are closely related. Here, the need is to provide modeling tools and assessment capabilities for tracking the dispersion of accidental or purposed release of toxic agents. Fluid modeling and computation fluid dynamics modeling are tools that have been identified to provide a basis for this requisite capability. These components provide synergism to the air quality modeling needs. Fluid modeling activities focused on characterizing the dispersion and transport associated with the collapse of the World Trade Center's twin towers. The information from the FMF studies provide an experimental bases for substantiating computational fluid dynamics (CFD) and subgrid scale modeling studies.

2.3.3 Urban Canopy Parameterizations

Urban canopy parameterizations (UCPs) are being developed and implemented in MM5 to improve fine-scale (~1-km grid spacing) simulations. The UCPs involve changes to the momentum and energy budgets in MM5, as well as acquisition and implementation of various databases of the urban morphology of the modeled cities. The UCPs in MM5 leverage the work of international scientists and contributions from visiting scientists and post-doctoral appointees.

In FY-2003, the UCP based on the drag-force approach (Lacser and Otte, 2002; Otte and Lacser, 2002) was applied to two July 1995 cases for Philadelphia. This UCP accounts for the drag exerted by urban structures, the increase of turbulent kinetic energy particularly near the tops of buildings, and the changes to the energy budget due to anthropogenic heating and the absorption and emission of radiation within the urban canopy (*i.e.*, from the surface to the tops of buildings). The MM5 simulations with the UCP for Philadelphia in the 1.3-km domain generate profiles of various fields that are more consistent with observations taken in urban areas, and resulted in better comparisons with meteorological measurements than the simulations that use the traditional methodology (roughness approach) in MM5 (Otte *et al.*, accepted for publication). These cases were also used to evaluate the impact of UCP-based fields on the CMAQ simulations, and special versions of MCIP were developed to include the effects of the UCPs on the PBL fields.

In addition, an advanced UCP that includes coupling with an urban soil model, SM2-U (Dupont *et al.*, accepted for publication)(a), was implemented in MM5 to add a more sophisticated and specific treatment of the energy balance in the urban areas as well as a treatment of vegetation and rural zones within the modeling domain. Initial tests of the advanced UCP in MM5 used the same Philadelphia test cases as the UCP described above, and those tests showed improvements in the MM5 simulation when using the urban soil model (Dupont *et al.*, accepted for publication)(b).

A more rigorous evaluation of the advanced UCP for Houston began in FY-2003. In preparation for the Texas 2000 modeling study, a detailed database of the urban morphology for Houston and the surrounding areas was purchased. Several key parameters were identified (*e.g.,* building density and height, vegetation density and height, plan area density, and many more). The processing of the morphology database was completed in mid-FY-2003. Sensitivities are planned for FY-2004 to determine the level of detail that will be required from an urban morphology database to have a positive impact on the meteorology and chemistry simulations.

2.3.4 Resolved Scale Modeling with CMAQ

Consideration of urban air toxic pollution is moving towards a community, exposure and risk-based modeling approach, with emphasis on assessing areas that experience elevated air toxic concentration levels, the so-called *hot spots*. Making these assessments will require characterizations of the spatial and temporal variability of toxic pollutant concentrations. Many toxic pollutants are active in photochemistry, and their ambient concentrations depend on regional background as the concentrations produced from local emissions. The CMAQ modeling system is being studied with the goal of producing pollutant features at high spatial resolution to drive exposure models. The effort starts by setting the nesting of CMAQ for modeling from regional to fine scales. Modeling results for various nests will be displayed and discussed. Given that exposure and risk assessments are typically focused on populations in urban and industrial areas, a review is made of the requirements for modeling meteorological and air pollution fields in urban areas at grid resolutions of the order 1 km. Subsequently, the 1.3-km grid simulations in CMAQ is utilized as a basis for examining the inherent within-grid spatial variability unresolved at native coarser scales. The examination reveals an additional sub-spatial grid variability at less than 1.3 km. The methodology to attain information at grid scales smaller than 1.3 km will require utilizing dispersion and transport modeled at a finer scale, and their outputs will be in the form of distribution functions to compliment the 1.3-km CMAQ simulations.

Simulations for this study were made on episodic bases and were focused on the Philadelphia area. MM5 and CMAQ simulations were performed using nests at 36-, 12-, 4-, and 1.3-km horizontal cell sizes and results are shown for July 12 and 14, 1995. At 1.3 km, urban canopy parameterizations (UCPs) were introduced into MM5 to account for the impact of urban building structures on the meteorological fields (Lacser and Otte, 2002; Dupont, *et al.*, 2003; and Ching *et al.*, 2003), based on Brown (2000) and Martelli *et al.* (2002). Sensitivity studies (not shown here) have shown pronounced affects of the UCP on both the outputs of the MM5 and the subsequent CMAQ simulations. The emissions were also spatially resolved at 1.3 km grids. Ten additional vertical layers were introduced into both MM5 and CMAQ to provide vertical resolution for implementing the UCP methodology. Studies showed some sensitivities to the layer or layers nearest the surface in which small point, area, and mobile sources were introduced.

Figure 10 displays the carbon monoxide (CO) distribution resulting from four nested CMAQ model grids. Using a smaller grid size enhances the spatial structure (gradients) and the peak concentrations. The impact on such photochemically active compounds as ozone is even more pronounced. To investigate the sensitivity of the simulations to grid resolution, a simulation made at 1.3-km grid cells was established as a base case and ozone concentrations were aggregated to grids corresponding to coarser grid resolutions. Aggregating the model results in this manner also enables study of the within-grid variability. Figure 11 compares the 1.3-km ozone concentration simulated at 4 p.m. (EDT) with the 12-km aggregated concentration. This limited set of model runs show:

- Introducing UCPs into the model changes the modeled flow and the resulting air quality fields;
- Resolving the flow and air quality at fine scales will significantly increase the level of detail in the spatial features, increase the intensity of the concentration gradients, and increase peak values; and
- Compositing neighborhood scale simulations to coarser scales yields different results when compared to coarse grid native simulations; the fine scale grid simulations provide indications of variability in coarser grid solutions; and the character of these results differs depending on the scale of the coarse grid mesh.

During FY-2004, this effort will continue with runs of an air toxics version of CMAQ with 12- and 4-km horizontal cell sizes and for subset of runs at 1-km grid spaciang focused on the Philadelphia and Delaware areas on an annual basis. These sets of simulation will be used to provide inputs for human exposure assessments that require annual ambient concentration values. Future studies will focus on detailed meteorological and air quality simulations using the high resolution gridded UCP for Houston.

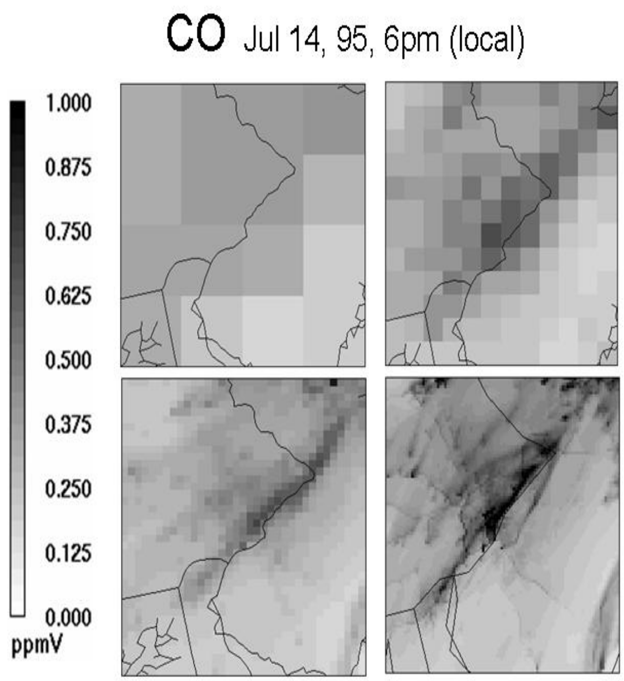

Figure 10. CMAQ simulations of CO at different spatial resolutions centered over Philadelphia. Top (left: 36km, right: 12 km), Bottom (left: 4 km, right: 1.3km)

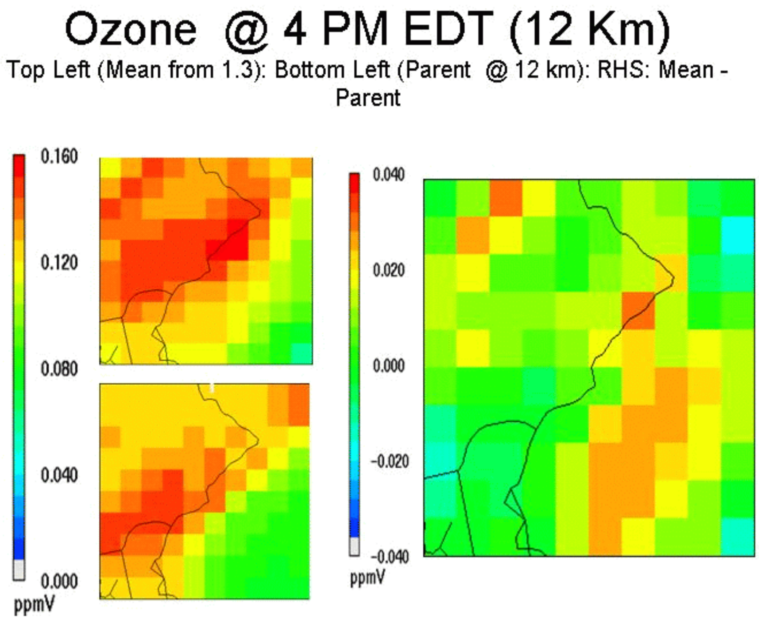

Figure 11. Ozone at 4 pm EDT (12 km).

2.3.5 Modeling Subgrid Concentration Variability

To improve human exposure and risk assessment modeling tools in urban settings, within-grid concentration variability distribution functions in the form of probability density functions (PDFs) are needed to complement finely-resolved scale (~1 km) model outputs. When considered in the context of human exposure modeling and risk impacts, the within-grid spatial variability in concentration fields arising from the distribution of sources in each grid can be as important, and in many instances perhaps even more important, than the grid resolved fields. For this research, the subgrid variability (SGV) from photochemistry and source dispersion processes were considered. The goal is to develop PDFs that will incorporate contributions from (1) multiple source dispersion and (2) from turbulence-induced photochemistry SGV derived from a large-eddy simulation model with direct chemistry coupling using the LESChem model of Herwehe (2000).

During FY-2003, efforts began to formulate distribution functions to represent the subgrid variability fields. In an exploratory phase, results from 1.3 km grid-resolved fields served as a surrogate for data at fine scales. These simulations were used to represent the subgrid scale variability for grid meshes of 4 km and 12 km, recognizing that this approach will be refined when modeling results from the source distributions and from subgrid chemistry become available. The figures provide illustrative statistics to demonstrate the qualitative aspects of such distributions. Figure 12 shows the standard deviation of the within grid variability at 4 km and 12 km. Figure 13 displays that the distributions for each of the pollutants exhibit a wide range in the value and sign of its skewness. Since exposure estimates depend on concentration and dosage, the magnitude of the range of the within grid variability becomes an important measure of risk. Figure 14 shows the range computed from the difference in the peak and minimum values of the 1.3 km results for each cell of the 12- and 4- km simulations normalized by their respective coarse scale aggregated grid mean. For the central Philadelphia area, the range exceeds the mean by up to a factor of 2.

Figure 15 depicts concentration distribution histograms from CMAQ simulations for a 12 km grid from the 1.3-km grid simulations centered on Philadelphia for 17-20 GMT, July 14, 1995. Here the histograms can change rapidly in time, and their characteristics also differ between the different pollutants. Several of the distributions exhibit multimode character and such shapes changes in time.

From this limited set of model runs, a few noteworthy points emerge. The degree of within grid variability varies as a function of grid resolution and pollutant species. The characteristics of this variability depend on many factors, including the complexity of the urban area and the distribution of emission sources. Even as the grid mesh resolution is refined to 1 km or less, within-grid variability will generally occur due to within grid source configurations and distribution and to chemistry and turbulent interactions (Ching *et al.*, 2003). Methods to describe these distributions will be a key focus during FY-2004. The fine-scale modeling results also have implications in assessing model evaluation. In some areas, within grid air concentration distributions may exhibit an inherently high degree of spatial variability throughout a model domain; a comparison of model results with observations should factor-in such variability. In general, since monitors will not be adequately sited to represent the grid resolved value, model comparison and evaluation should introduce some measure of this subgrid scale variability.

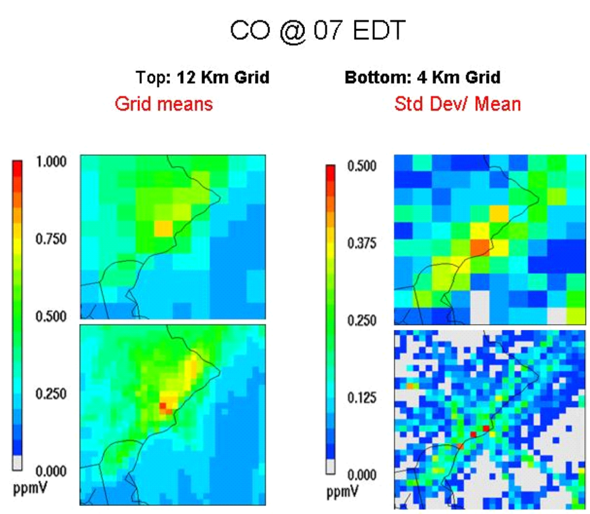

Figure 12. CMAQ simulations of CO for July 12, 1995.

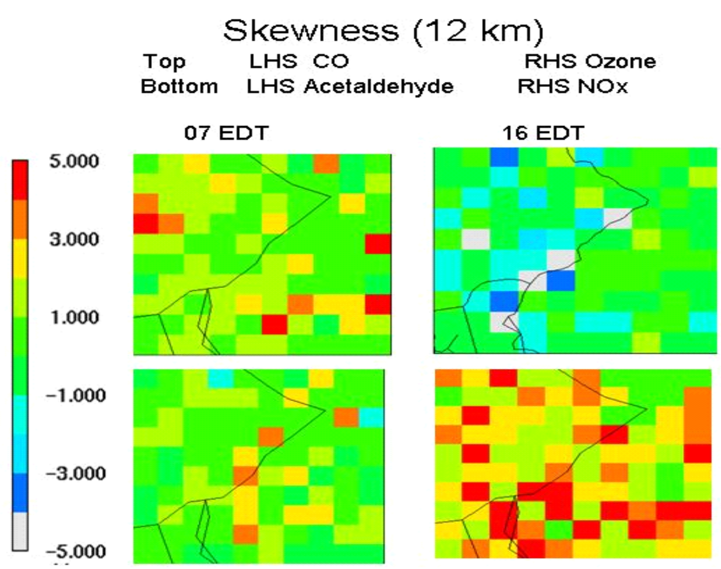

Figure 13. Skewness at 12-km grid resolution derived from 1.3 km simulations for July 12, 1995.

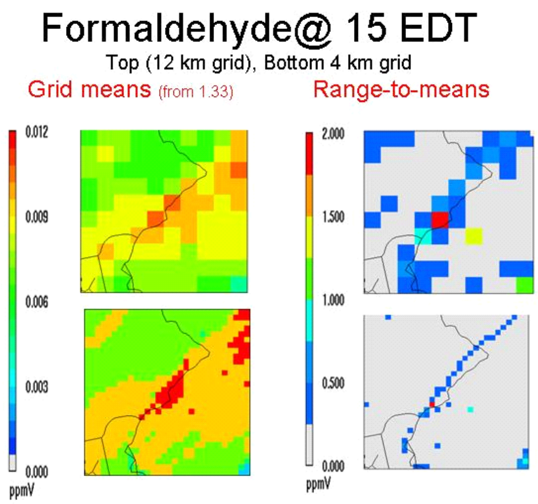

Figure 14. Grid and range-to-mean derived from 1.3-km CMAQ simulations of formaldehyde for July 12, 1995.

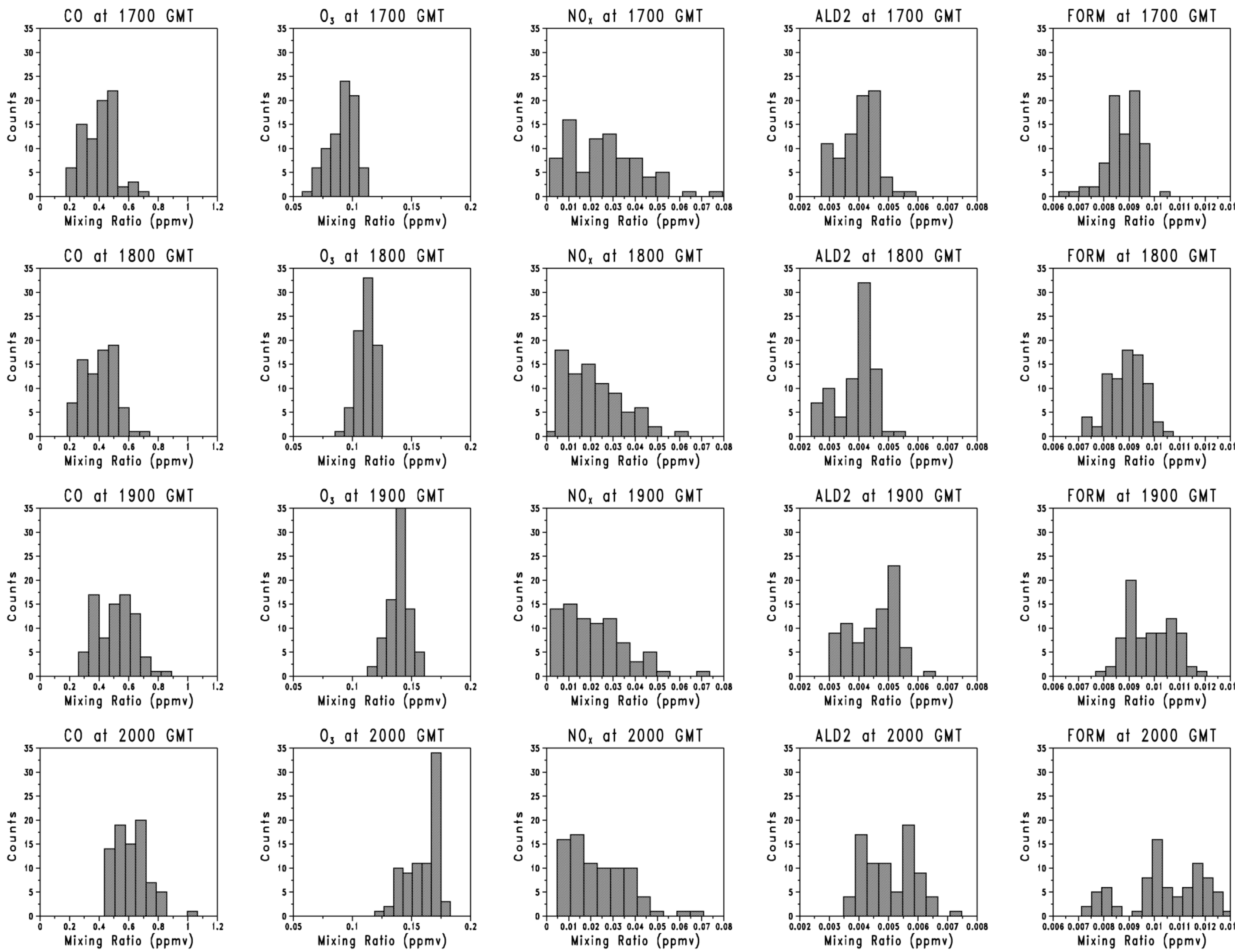

Figure 15. Concentration distribution histogram for 12 km cell in Central Philadelophia. From left, CO, 0_3, NO_x, acetaldehyde and formaldehyde. From top, 1700, 1800, 1900, and 2000 GMT.

2.3.6 Wind Tunnel Modeling of the World Trade Center Disaster Site

The September 11, 2001, destruction of the World Trade Center (WTC) in New York City resulted in the release of a large volume of airborne pollutants in the form of fugitive PM and various combustion products. These emissions persisted at varying degrees for weeks and months after the initial catastrophic event. This event has elevated the need for reliable models to predict concentrations of such contaminants in complex urban areas. To improve our understanding of the transport and fate of pollutants emitted at the WTC disaster site, a laboratory study was initiated in FY-2002 and continued through FY-2003 in the Fluid Modeling Facility's meteorological wind tunnel using a 1:600 scale model of Lower Manhattan. The results of the study will be used to evaluate and enhance our numerical simulation capabilities for Lower Manhattan and other urban areas and to support ongoing risk assessment and public health studies of the WTC disaster.

The wind tunnel study included measurements and visualizations of flow and dispersion for three wind directions (315°, 270° and 225°) relevant to the climatology of Lower Manhattan in late autumn. Flow visualization was accomplished by illuminating theatrical smoke released from the WTC site to develop a qualitative description of plume dispersion and highlight the general flow features. Concentration measurements of a tracer released from the WTC site were performed to quantitatively describe the spread of the plume as it interacted with the complex building geometries of this highly urban area. Flow measurements were made using Laser Doppler Velocimetry (LDV) to examine in detail both the mean flow and turbulence levels within the street canyons. Selected results for the westerly (270°) wind direction are presented here.

In the flow visualization phase of the experiments, a laser light sheet was used to reveal the extent and structure of the cross section of the plume at various locations across the city. One of the most prominent features observed was the entrainment of source material by the tallest buildings around the WTC site. This upwash or ventilation of smoke along the lee side of these buildings brought material up to and above the building tops providing initial vertical mixing and elevated release of the WTC pollutants. This phenomenon is shown in Figure 16 in the lee of three dominant Lower Manhattan buildings (the World Financial Center, Liberty Plaza, and Chase Manhattan) where the horizontal laser sheet illuminates three elevated plumes. Additionally, large clusters of tall buildings, as found in the Wall Street area to the south and east of the WTC site, function as single large obstructions to the flow. During the smoke visualization, plume material moving eastward deflected toward the south around the Wall Street area. The surface-level concentration distribution for the 270° wind is displayed in Figure 17. As observed qualitatively in the flow visualizations, the concentration measurements show the plume moves initially toward the east, and eventually wraps around the Wall Street cluster of buildings. Near the WTC site, the plume shows significant crosswind and even upwind spread due to the mixing and updrafts caused by the buildings surrounding the site. The values of concentration in Figure 17 and Figure 18 are non-dimensionalized as $100CUH^2/Q$, where C is tracer concentration, U is free-stream speed, H is the urban height scale (90 m full scale) indicative of the average building height, and Q is the volumetric source flow rate.

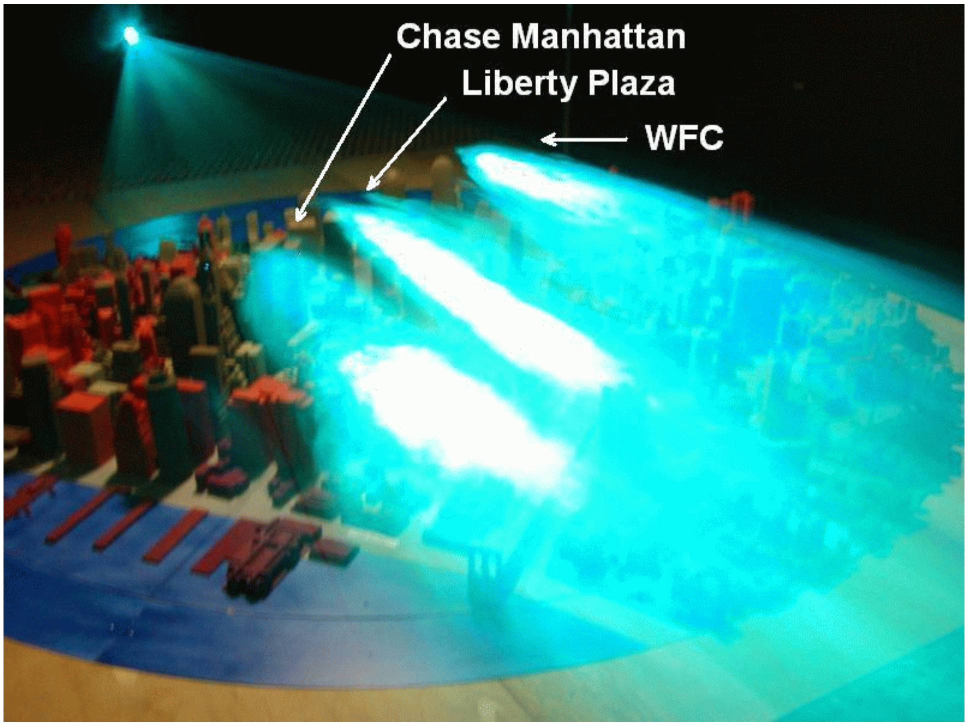

Figure 16. Smoke released from the scale model of the rubble pile at the WTC site enhanced by horizontal sheet of laser light at elevation just above tops of tallest buildings. Wind direction is westerly.

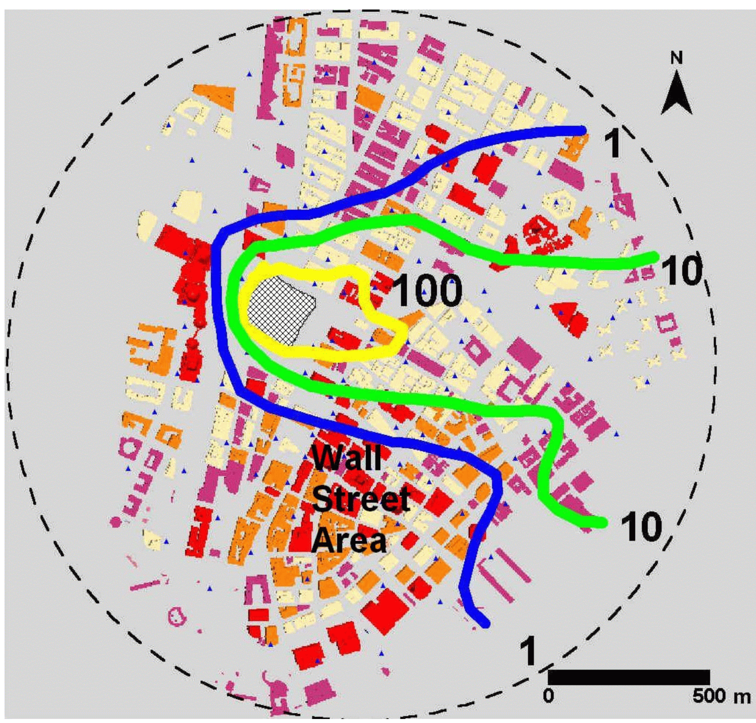

Figure 17. Surface concentration pattern in the scale model of Lower Manhattan for the westerly wind direction.

(Tab) In addition to the surface measurements, vertical slices of plume concentration were measured at 300, 600, and 1200 meters (full scale) downwind from the WTC site. Figure 18 depicts these cross sections against the background of the city skyline, as viewed from a downwind position looking into the wind (looking westward). The measurements again support the observations of the smoke visualization. At 300 meters (about 3 city blocks) downwind, the plume cross section (Figure 18a) exhibits a double lobe in the 10 and 1 contours reflecting the near source upwash of material from the Liberty Plaza building to the south and the World Financial building to the northwest. At 600 meters (Figure 18b), the double lobe is still apparent but the plume and its peak concentration have shifted toward the south. This is the beginning of the blocking and deflection effect of the tall, dense cluster of buildings in the Wall Street area. At 1200 meters (Figure 18c), the plume continues to grow and shift toward the south. This represents the plume distribution that is leaving Manhattan and is available for transport to downwind locations (*i.e*. Brooklyn, Long Island, etc.).

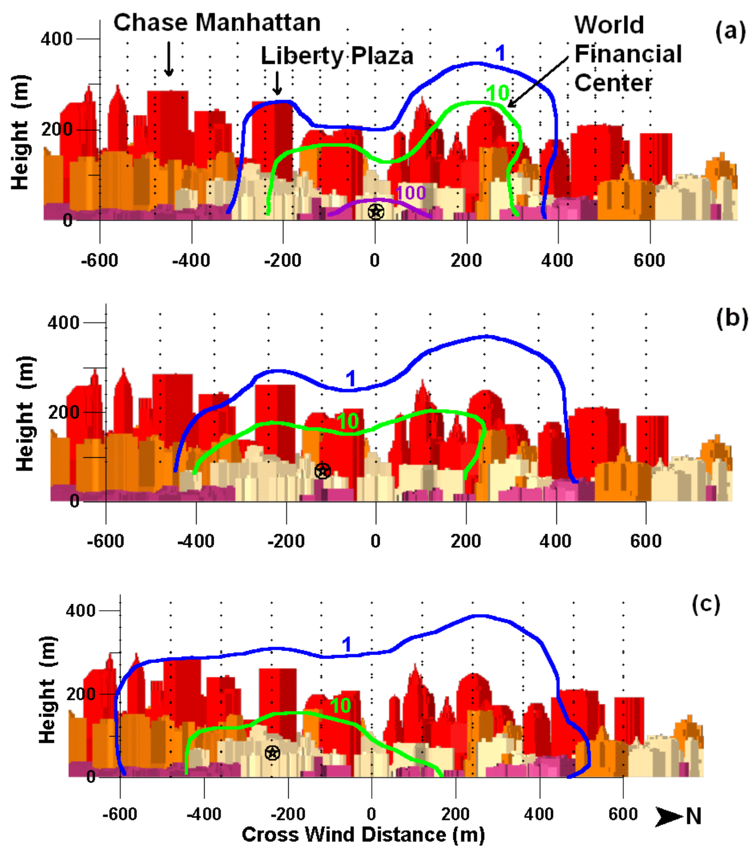

Figure 18. Plume cross sections at downwind distances of: a) 300 m, b) 600 m, and c) 1200 m from the rubble pile for the westerly wind direction. The view is directly upstream against skyline of the city. Colors indicate categories of building heights.

Understanding the local dispersion of contaminants within the complex urban canopy of Lower Manhattan requires flow characterization within and above the wide variety of street canyon geometries. Velocity and turbulence fields were sampled using LDV, a non-invasive technique where, in this study, laser beams were projected through optical quality windows in the floor of the wind tunnel. The measurements show that the flow generally follows the street canyons at elevations below the local roof lines, even in streets that are aligned as much as 60° from the free-stream wind direction. As elevation increases, the flow tends to align with the free-stream direction except in the vicinity of the taller buildings.

One of the street canyons that was examined in some detail is three to four blocks northeast of the World Trade Center site on Church Street near the transition from areas of low and medium rise buildings. Flow in planes perpendicular to Church Street is shown in Figure 19. These cross sections are located only 60 m (one block) apart along Church Street and are separated by a cross street (Murray Street). In Figure 19a, with the upwind and downwind buildings at about the same height, the flow appears to recirculate within the street canyon. There is also a velocity component along the street (not shown) such that the flow actually spirals up the street. In contrast, only one block away a much taller building stands upwind and no spiraling or recirculating flow is evident (Figure 19b); instead, upwash on the lee side of the upwind building is very strong over the entire width of the street. This example of the complexity of the flow fields in Lower Manhattan and the variability over very short distances illustrates the challenge that modelers have in quantifying the transport and fate of airborne pollutants in major urban areas.

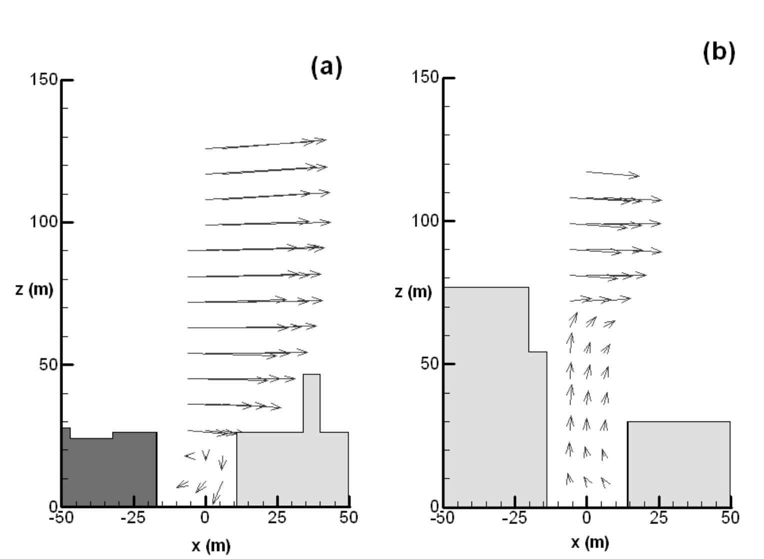

Figure 19. Flow patterns along Church Street for the westerly wind direction, three to four blocks northeast of the WTC site, illustrating complex flows in street canyons.

Wind-tunnel measurements of velocities and dispersion have demonstrated the complexity of the flow field in and above the street canyons of Lower Manhattan. However complex, there are several generalities of the flow and pollutant dispersion that can be deduced from this study and consequently considered for testing against numerical modeling approaches. The manner in which areas of densely-packed buildings act as obstructions to the flow and the manner in which tall buildings can quickly move pollutants near the surface to high elevations are just two examples. Aside from improving numerical modeling tools for general air pollution and homeland security type applications, laboratory data can be useful for developing guidelines for emergency responders making critical evacuation decisions. The model of Lower Manhattan will be used in future studies to examine other release locations and release types in a variety of street canyons and intersections.

2.3.7 Numerical Modeling of the World Trade Center Site

The scope of ongoing numerical modeling in support of the environmental assessment of the events at the WTC during and subsequent to September 11, 2001, has three principal components: (1) meteorology and pollutant plume in the New York Metropolitan Area and impact on downwind locations, (2) fine-scale pollution impact in the local area of Lower Manhattan south of Canal Street, and (3) assessment of human exposure to ambient pollution. Actual emission rates of pollutants from "ground zero" are unknown; therefore, models cannot be applied to estimate pollutant levels.

A general characterization was completed of the dispersion of particulate matter from the WTC recovery site in the ambient air during the three months following the September 11, 2001, events. Hourly estimates of plume transport and unit source dilution were made using a blended observational and dispersion modeling approach. A derivative of the CALMET-CALPUFF dispersion model was employed to simulate the plume dilution for a 50-km x 50-km square area surrounding Lower Manhattan. This modeling was completed in collaboration with the North Carolina State Climate Office, North Carolina State University, Raleigh, North Carolina. Figure 20 displays an example plume mapping, which is representative of a single 1-hour plume. Figure 21 displays the time average of the 1-hour plumes and the wind rose for the September 11–13 period. The plume color code represents the estimated dilution. Local wind flow patterns caused by the sizable buildings in Lower Manhattan are not considered here. Hence, these plume simulations can be considered appropriate for distances beyond 2 km downwind of the WTC site.

Computational Fluid Dynamics (CFD) simulation methods are being developed to better estimate fine-scale flow patterns and pollutant dispersion. A digital model of the buildings of Lower Manhattan are necessary to support the set up of a CFD simulation. A digital model replication of all buildings south of Canal Street in Lower Manhattan was developed using licensed digital information from Vexcel Corporation. A digital model of each building was developed to support construction for wind tunnel model studies and the computation fluid dynamics numerical simulations studies of the fine-scale pollution dispersion. Figure 22 shows a CFD simulation of the winds and potential pollution transport pathways (streamlines) for westerly winds. The wind tunnel model study of the same area is providing data on the winds and pollution transport. Information from the wind tunnel model study will be used to develop and evaluate the numerical simulation models for the buildings of Lower Manhattan. In addition, the CFD simulation methods are being developed and evaluated by examining comparisons with a range of past idealized wind tunnel model studies. Once these evaluation studies are completed, the numerical simulations can be extended to a wider range of situations and meteorological conditions. In addition, a CFD model was set up for simulating the collapse of the North Tower. The collapsing tower was modeled by "pancaking" the building floors under the force of gravity. The resulting simulated wind speeds exceeded 100 mph at the base of the collapsed tower where vortices are generated and radiated outward carrying smoke and dust just as was observed. Figure 23 depicts the outline of the resulting smoke/dust plume. Ongoing developments include adding different mass (weight) particles to CFD simulation of particle transport and dispersion for comparison with available information of the deposition pattern around the WTC site.

A Division scientist participated in a workshop on environmental monitoring and modeling associated with national emergencies to examine what was learned following the events of September 11, 2001, at the New York City World Trade Center, and potential response if a similar event occurred. Models exist to help general understanding of pollution transport on a metropolitan to regional scale. On these scales, modeling information combined with air monitoring information enables the assessment of where and when potential emissions may affect people. Rapid responses using these models are possible when a real-time meteorological measurements and demographics information are immediately available. New techniques are needed to improve fine-scale pollution transport near the source and within the neighboring building environments. Further research and development is needed to adapt existing exposure models for emergency scenarios. For acute exposure assessments, models need to be developed based on microenvironmental (*e.g.*, outdoor and indoor) concentration fluctuations and exposure variability for different media (*e.g.*,water, air, soil, dust, food, sediment). For chronic exposure, models need to be developed based on microenvironmental average concentration and people's activities and locations relative to the source.

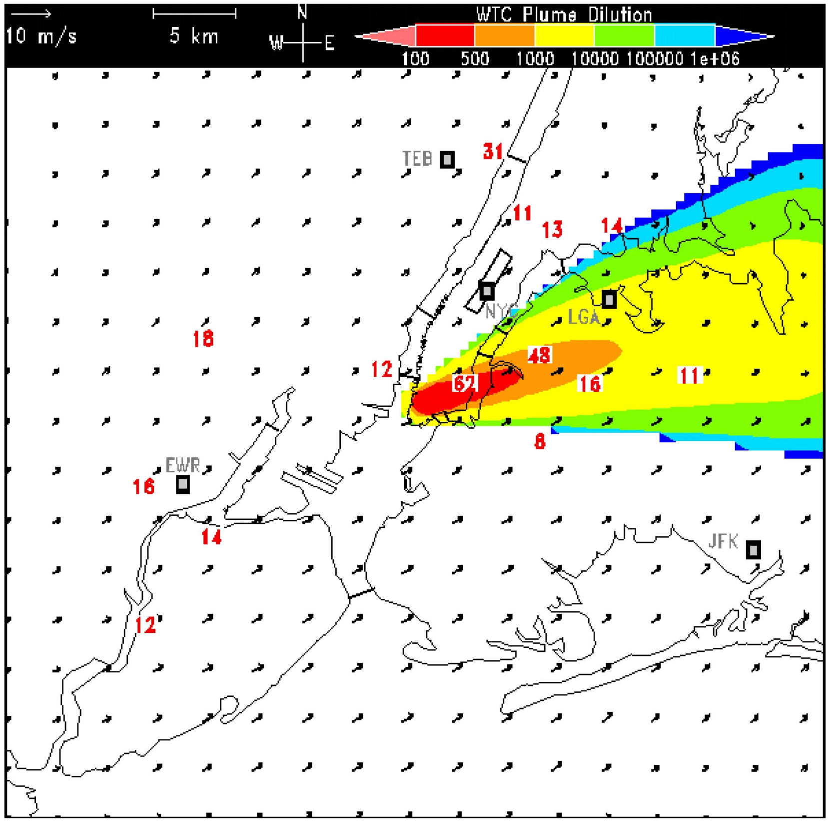

Figure 20. Simulated CALPUFF dilution of a volume source located at the WTC. Numbers are hourly-averaged $PM_{2.5}$ concentrations.

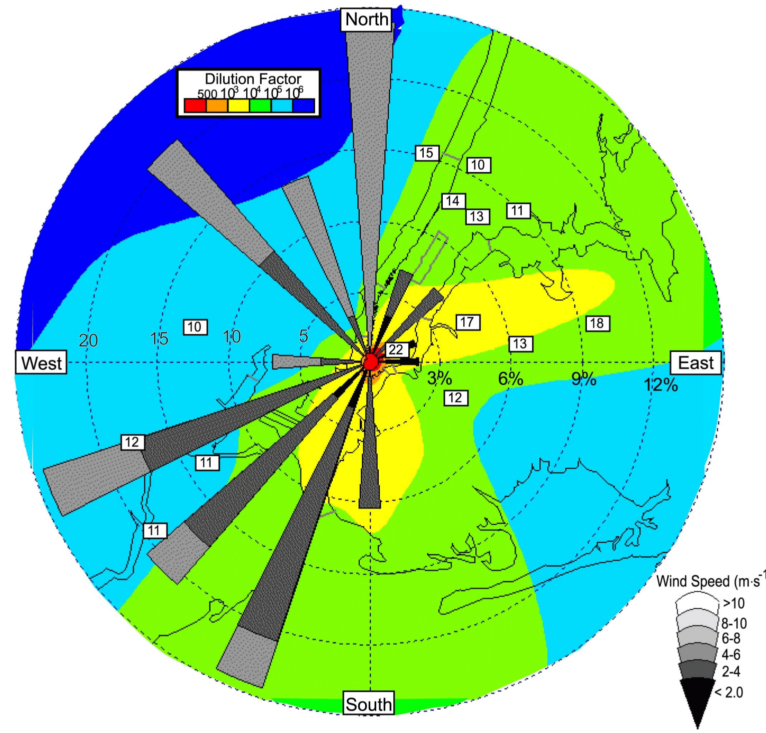

Figure 21. Wind rose, dilution map, $PM_{2.5}$ concentrations for average over the period September 11-13, 2001. Wind rose for the gridpoint closest to the WTC.

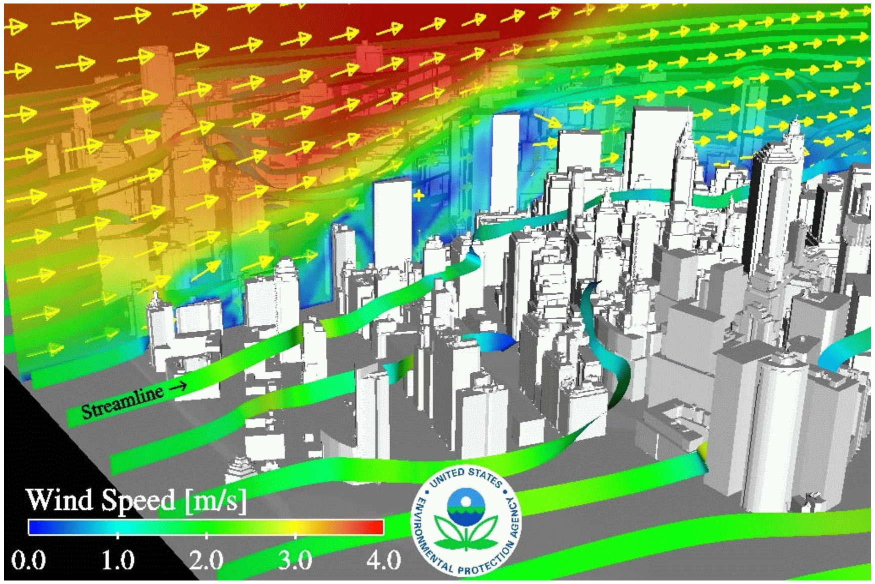

Figure 22. CFD winds and streamlines through Manhattan street canyons.

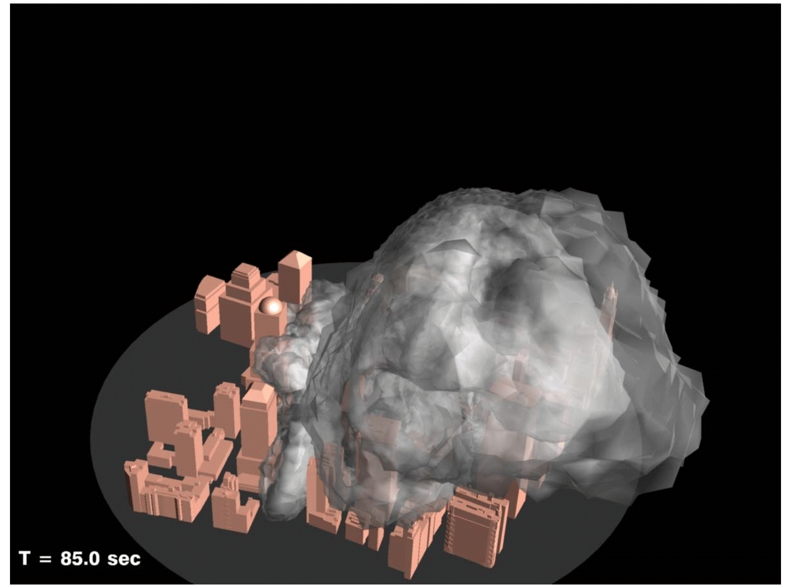

Figure 23. CFD simulation of smoke and dust cloud following (Tim=85 sec) the collapse of the North Tower.

2.3.8 Development of Compartmental Modeling Tools for Toxics

The release, transformation, transport, and environmental fate of toxic pollutants are an inherently multimedia chain of events. FY-2003, multimedia research regarding fully coupled, multimedia, dynamic, hybrid compartmental models, focused on the expansion of the 3cm pilot compartmental modeling tool under the MIMS framework. Programming support was provided by the Argonne National Laboratory (ANL) and consultative assistance was provided by Multimedia Envirosoft Corporation, Los Angeles, California. The Four Compartment Hybrid Model (4cm) application builds, solves, and displays the results of a system of coupled ordinary differential equations (ODEs) and partial differential equations (PDEs), describing the dynamic movement of chemical mass through multiple media. Like the 3cm, the 4cm was implemented under the MIMS framework.

The 4cm multimedia system includes uniform air, water, and biota (fish) compartments as well as a relatively simple non-uniform mixed-phase sediment compartment. The initial test case developed for the 3cm was repeated for the 4cm and follows the movement of chlorobenzene, a volatile organic chemical used as a solvent and in the production of other chemicals, through air and water media to Alewife (prey) and Salmon (predator) endpoints. The initial simulation period spans 3-summer months (~2160 hours) for a water body with geographic characteristics similar to Lake Michigan and climatological conditions similar to Detroit, Michigan. Like the 3cm, the 4cm is not intended to accurately reproduce observed chemical concentrations, but to 1) test the ability to implement the modeling approach under the MIMS framework, 2) begin modification of an existing commercial model configuration, MEND-TOX (Cohen and Cooter, 2002a; 2002b) to facilitate integration with air quality model development research, and 3) demonstrate the practical, in-house, *i.e.*, no proprietary code, implementation of the unique PDE/ODE coupling approach developed by Cohen. In addition to development of the coupling algorithm, the 4cm requires additional expressions accommodating aqueous as well as solid phase chemical movement within and out of the sediment medium.

Implementation of the coupled hybrid compartmental approach proved more challenging then originally anticipated. Tasks associated with model development included identification and testing of a simple, fast PDE solution routine and modification of the ANL DIAS©®[4] (Dynamic Information Architecture System) and MIMS frameworks. The resulting pilot model remains unacceptably slow in its present form, but its development has facilitated in-house understanding of uniform and non-uniform media coupling such that these lessons-learned can now be applied, where appropriate, to future multimedia CMAQ model research and development, *e.g.*, regional-scale natural emission, transformation, transport, deposition and re-emission of Hg.

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[4]Copyright of Argonne National Laboratory. "Dynamic Information Architecture System" by John H. Christiansen, and A. Peter Campbell. U.S. Patent # 6058387 (2 May 2000).

2.4 Multimedia Modeling

2.4.1 Multimedia Integrated Modeling System

ASMD continued development of the Multimedia Integrated Modeling System (MIMS), which includes the MIMS framework and the spatial allocator. The MIMS framework provides a software infrastructure to support configuring, applying, and evaluating environmental models. ASMD enhanced the framework to make it easier to set up complex simulations, for instance, where models are invoked repetitively or where there are many input or output parameters. A Java scientific plotting library (based on the open source statistical package R) was also significantly enhanced. OAQPS released its first version of the Total Risk Integrated Methodology (TRIM) multimedia modeling system based on MIMS, which provides scientific graphics and execution configuration and management support for TRIM. Another group used MIMS as the basis for a prototype decision support system. The decision support system uses nonlinear optimization to find promising alternatives that balance economic and environmental objectives. In that system, MIMS provides the infrastructure for user interaction and managing multiple model executions, which are used to explore the decision space.

The MIMS spatial allocator computes how spatial fields described on one set of polygons on the Earth's surface would be distributed to a second set of polygons. Examples of this type of operation include regridding and applying gridded model results and political boundaries. The spatial allocator permits the performance of these calculations with common environmental file formats without relying on a geographic information system. ASMD extended the spatial allocator to provide more complete support for air quality emissions processing. A number of groups were using the spatial allocator for that application.

2.4.2 Urban Drainage Decision Support System Prototype

A 2-year cooperative agreement was awarded in FY-2002 to develop and test the integration of the Storm Water Management Model (SWMM) with decision support tools to identify cost-effective and reliable watershed management strategies. A team of scientists from MCNC Environmental Programs, North Carolina State University, and University of North Carolina at Chapel Hill are the recipients of the cooperative agreement. The team is using the MIMS framework as an integration platform for developing the prototype urban watershed decision support tools. The prototype is being designed with local and city planners who manage urban-point and non-point sources as potential users.

During the first year of the cooperative agreement, work was underway to design and implement the decision support and analysis tools. Included are such uncertainty analysis tools as a Monte Carlo and Latin Hypercube approach for uncertainty propagation, importance sampling, and uncertainty importance estimation. During FY-2003, these uncertainty and optimization tools were integrated into the MIMS framework for use with SWMM and other models within MIMS. Integration of SWMM with the uncertainty and optimization tools was also completed during FY-2003, along with tests of the coupled system in a case study of Rouge River near Detroit, Michigan. During FY-2004, this work will be completed by developing software interface tools for users less familiar with the decision support and analysis tools.

2.4.3 MultiLayer BioChemical Model—Area Weighted

CASTNet is operated by the EPA Clean Air Markets Division (CAMD) and the National Park Service to monitor concentration and dry deposition at sites across the country to assess long-term trends in air quality and environmental protection resulting from regulatory policies and emission reductions required under the Clean Air Act. CASTNet estimates dry deposition flux by combining measured concentrations of pollutants with modeled deposition velocities. In FY-2000, an evaluation was performed of the deposition velocity model MultiLayer Model (MLM) used by CASTNet, which identified several opportunities for improvement in the model. Over the last three years, a new deposition model was developed called the Multi-Layer Biochemical Model (MLBC), which addressed many of the weaknesses in MLM. The MLBC was described and evaluated in a series of published papers (Wu *et al.*, 2003a; 2003b). In the original design, MLBC treats all canopies as a mixture of the plant species. For CASTNet, the canopy at a site is treated as spatially distinct species where the deposition velocity is determined from area weighting the deposition velocities for each of the local species. MLBCv1.0 is being modified to allow for this latter approach to develop a new version of the model, which will be referred to as MLBC-AW (Area Weighted) to denote the area weighting algorithm. Additionally, both the MLM and the MLBC will be integrated into the MIMS framework to facilitate this comparison as well as create an easier framework for CAMD and its clients to run the models with CASTNet or other data.

2.4.4 Chesapeake Bay 2006 Re-Evaluation

ASMD has established a long-term relationship with the EPA and NOAA Chesapeake Bay Programs to address multi-media environmental problems where the atmosphere is an important source of reduced and oxidized nitrogen through deposition. Chesapeake Bay is a leader in using multi-media modeling. Two major Chesapeake Bay re-evaluations or assessments of required nitrogen load reductions to the Bay have already occurred. The next re-evaluation is slated for 2006 or shortly thereafter.

Chesapeake Bay has been placed on EPA's list of impaired waters. The Chesapeake 2000 agreement calls for preempting the need for a TMDL (Total Maximum Daily Load) plan by cleaning up the Bay by 2010. The Bay 2006 re-evaluation is a critical step in this process towards the 2010 cleanup and delisting, and ASMD is participating in the re-evaluation process. The best science is desired for the re-evaluations, and during the period between major re-evaluations, ASMD is changing its multi-media modeling of nitrogen from the Extended RADM to its new model, CMAQ. CMAQ has been sufficiently evaluated for deposition to show that it is an improvement over the Extended RADM. A newly designed aggregation data set with 40 cases was developed for CMAQ that can directly address seasonal deposition, an improvement over the older aggregation set. The outer, continental grid resolution is 36-km, a significant reduction over the 80-km resolution used with the Extended RADM. For Chesapeake Bay multi-media simulations, a 12-km nest over the Mid-Atlantic region covering most of the Chesapeake Bay airshed was developed. This inner nest better resolves the Bay surface compared to the 20-km nest used with the Extended RADM. The MM5 meteorological runs for the 36-km aggregation set and the 12-km nest were completed during FY-2002. Prior to establishing new base cases with CMAQ, testing is now underway to determine the best method for parameterizing the mixing height, because the CMAQ MCIP has new capabilities available. CMAQ dry deposition algorithms were revised in FY-2003, improving deposition parameterizations for NH_3, HNO_3 and other nitrogen containing species. CMAQ now tracks wet deposition of organic nitrates, which was omitted in the Extended RADM. Organic nitrates are estimated to be 10-20% of the wet nitrogen deposition budget and it is expected that a significant fraction of organic nitrates in rainwater could be products of photochemistry. An updated calculation of 1990 nitrogen deposition was completed in FY-2003 and will be compared to the previous estimates made using the Extended RADM.

2.4.5 Ammonia Budgets for Coastal Systems

An important fraction of atmospheric nitrogen deposition is reduced nitrogen (ammonia/ammonium). In the future, with successful implementation of the EPA regulations on NO_x emissions for control of ozone and increases in animal operations in the eastern seaboard states, reduced nitrogen is expected to become a majority of the nitrogen deposited from the atmosphere. However, ammonia is not receiving the attention it deserves, in part, because many ecologists dealing with marine estuaries and watersheds believe ammonia deposits instantly so that none leaves the immediate area. Long-range transport of ammonia is ignored. ASMD has an opportunity to correct this misinterpretation of data through modeling and model-data interpretation studies using the regional models. Model atmospheric budget analyses were performed in FY-2002 with MAQSIP, a development predecessor to CMAQ, for North Carolina ammonia emissions associated with the large increase in the hog population. The analysis, covering a short summer period and reported at the International N2001 Conference, show that only 5 to10 percent of the NH_x budget dry-deposits locally while most of the ammonia emissions are involved in long-range transport. This is contrary to conventional wisdom. The model results are consistent with spatial and temporal trends in the ammonia wet deposition data. A regional exploration of the ammonia budget was performed for the eastern United States using the Extended RADM (Mathur and Dennis, 2003). The conclusion thus far is that the conventional wisdom that assumes there is no long-range transport of ammonia is incorrect. Nonetheless, the conventional wisdom persists and distorts studies of nitrogen-cycling in coastal estuaries, introducing significant errors in them.

The 1999 summer period was chosen for the next phase of analysis due to availability of special 12-hour integrated gas and particle measurements at the Clinton site in the middle of the hog farm area in North Carolina. The ammonia inverse was re-applied to July and August 1999.

Test simulations were carried out at 32-km and 8-km resolutions with the newer CMAQ but with the older M3Dry deposition algorithms. Preliminary comparisons showed very reasonable agreement between modeled and measured NH_X levels at Clinton and Atlanta, Georgia. With the updated M3Dry deposition algorithms and with processes analysis turned on for budget studies, CMAQ runs are underway at the 8-km resolution to support the analysis.

2.4.6 Remote Sensing Image Processing: Pamlico Sound Study

The AVIRIS (Airborne Visible and InfraRed Imaging Spectrometer) was flown over Pamlico Sound, North Carolina, on May 15, 2002. In a coordinated effort involving EPA, NASA, NOAA, the University of North Carolina at Chapel Hill, University of Maryland, and Duke University, data were collected to characterize the spatial variation of chlorophyll A, suspended sediment, and colored, dissolved organic matter (CDOM)) across the Pamlico Sound using both hyperspectral remote sensing from 20 km above sea level, low altitude SeaWiFS simulator imagery, submerged radiometery, and chemical/biological analysis of water samples. At the request of EPA, NASA offered the services of the ER-2 flight mission team to fly the Pamlico Sound and Lower Neuse River Basin during a window from May 10 to June 5. Weather conditions on May 15 provided near-perfect atmospheric and surface conditions for the imaging.

The objective of atmospheric correction of remotely sensed imagery is to derive surface reflectance (*i.e*. spectral albedo) from measured upwelling radiance. The method employed here used a look-up table approach, whereby MODTRAN (MODerate resolution radiative TRANsfer model) is used to generate tables of radiances from known reflectance surfaces and model atmospheres of known precipitable water vapor and aerosol optical depth. The inverse problem (radiance-to-reflectance) is solved by referencing the appropriate tables. The correction converted the measured upwelling radiance from 370 nm to 2510 nm to reflectance by removing the degrading effects of atmospheric attenuation and scattering when viewing the ground from 20 km altitude (Figure 24). The spatial precision of the correction was scene-wise (approximately 50 km x 50 km) for atmospheric gasses, pixel-wise (20 m x 20 m) for water vapor, and approximately 100 m x 100 m (variable) spatial precision for aerosol correction.

A dark surface water vapor algorithm was developed and tested in the latest iteration of a reflectance processor model. Dark surface aerosol algorithms from recently published literature (Kahn *et al.*, 2001; Holben *et al.*, 1998) will be incorporated. These enhancements will enable accurate determination of the atmospheric water vapor fields and aerosol optical depth over class II waters such as the Pamlico, and yield improved accuracy in surface reflectance.

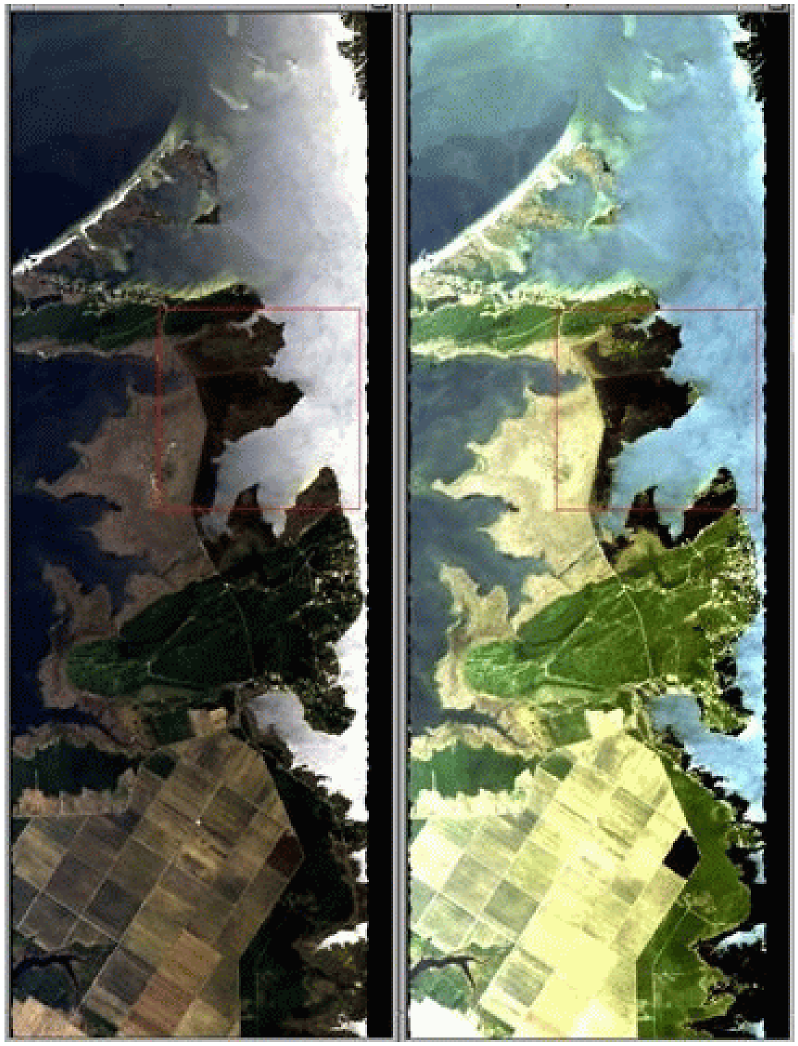

Figure 24. The image on the left displays raw radiance from the AVIRIS spectrometer. The same image on the right is shown as surface reflectance, following glint- and atmospheric correction.

2.5 Climate Change Impacts on Regional Air Quality

The Climate Change on Regional Air Quality (CIRAQ) project was initiated in FY-2002 and will directly contribute to the EPA Global Change Research Program's (EPA GCRP) assessment reports of global climate change impacts on air quality. The Division's role in the assessment is to simulate air quality on a national domain under current and future climate change conditions. The planned products for this effort are designed to provide results and analysis in a timely manner for the EPA GCRP 2007 air quality assessment report. Current and future (2050) 10-year regional climate simulations are under development during FY-2003-04 and will be followed by CMAQ air quality simulations during FY-2004-06. The primary goal of these simulations is to develop future air quality modeling scenarios to compare against current conditions to test the sensitivity of air quality to potential climate change. During FY-2003, CIRAQ activities included:

Regional climate downscaling of meteorology. To support this project and ultimately the air quality assessment, the EPA GCRP is funding the Department of Energy's (DOE) Pacific Northwest National Laboratory (PNNL) to develop current and future regional climate simulations. These simulations will rely on MM5 with initial and boundary conditions from global climate model (GCM) simulations, and the future GCM simulations will be rely on Intergovernmental Panel on Climate Change (IPCC) future greenhouse gas scenarios. For comparison against observationally-constrained boundary conditions, MM5 simulations using NCEP reanalyzed meteorological fields as boundary conditions would also be performed.

During FY-2003, 10-year MM5 simulations using NCEP reanalysis fields as boundary conditions were completed (1990-2000) and transferred to ASMD for archiving. PNNL is in the process of completing two additional MM5 regional climate modeling simulations with boundary condition links to the National Aeronautics and Space Administration (NASA) Goddard Institute for Space Studies (GISS) GCM and the NCAR/PNNL Parallel Climate Model (PCM). These MM5 simulations using GCM boundary conditions will be compared to the MM5-NCEP results as a benchmark. MM5-GISS and MM5-PCM simulations will be performed for a reference period (*e.g.*, 1995 ± 5 years) and a future period under climate change conditions (*e.g.*, 2050 ± 5 years). As regional climate modeling simulations become available, ASMD regularly archives the data and develops the model-ready meteorology fields needed for CMAQ and the emissions processor SMOKE©.

Global climate and chemical transport simulations. During FY-2003, test simulations were performed with the NASA GISS GCM under a future IPCC greenhouse gas emission scenario. Ozone chemistry was also included in the simulation to provide chemical boundary conditions for CMAQ. The GISS GCM output from the present through 2050 will be analyzed to test how many years of CMAQ simulation are needed to separate out the influence of climate change trends from interannual variability. The GISS simulations include passive tracers to follow stagnation events in addition to a standard analysis of temperature and mixing height changes. Results from this analysis will be used to finalize the decision regarding the number of years of CMAQ simulation necessary for the analysis of climate change impacts on air quality.

EPA grant collaborations. In FY-2003, EPA Science to Achieve Results (STAR) grants and cooperative agreements were awarded to several groups focusing on global and regional air quality impacts from climate change. ASMD has established collaborative plans with four groups, including Harvard University, Carnegie Mellon University, and University of Illinois. Areas of collaboration include linkage of global chemical transport model results from different global models with CMAQ and evaluation of regional versus global results over the United States domain using methods such as empirical orthogonal functions. These activities will be ongoing during FY-2004, followed by the development of model-ready emissions for CMAQ based on emission factors for current conditions and the regional climate simulations for current and future periods. CMAQ simulations for the first incremental analysis of global climate change effects on air quality without future air quality emission scenarios will then be performed and analyzed during FY-2005–07 for the 2007 EPA GCRP assessment report.

Methods developed for analysis and evaluation of regional climate simulations. As MM5 regional climate simulation results become available for current time periods, it will be necessary to evaluate historical time periods against meteorology to assess the model performance. While it is not possible to evaluate future simulations against observations, the CIRAQ team developed tools to screen the MM5-GISS and MM5-PCM future results for outliers or unstable, non-physical results. The screening tools were tested and completed in FY-2003 and are being applied to the regional climate simulation results as part of the model-ready meteorology processing. Tools were developed to evaluate historical MM5 simulations against a suite of observations and generate graphs using GraDs.

In addition to direct evaluation of point observations at collocated MM5 grids, analysis methods developed to consider the spatial and temporal variations in the MM5 were tested. A cluster analysis method following Cohn *et al.* (2001) was implemented where major modes of spatial variability are identified from meteorological simulations. This method is helpful in comparison of spatial differences between simulations and against analyzed fields where observational data were assimilated. Meteorological fields known to be related to air quality will be considered using this method. Based on results from the cluster analyses, the Kolmogorov-Zurbenko (KZ) filter that was tested during 2003 for time filtering can be applied to spatial areas of interest. The KZ filter can separate out variations in meteorological variations into different time scales. With a 10-year simulation, it will be possible to consider daily, synoptic, seasonal, and interannual variations. Using time series analysis may help to identify differences between periodic variations and actual trends in climate. Both the cluster analysis and KZ filter methods can also be used to analyze air quality predictions once CMAQ simulations are completed.

2.6 Specialized Client Support

2.6.1 Assistance to State/Local Air Quality Forecasters

The EPA AIRNow program collects and disseminates Air Quality Index (AQI) data and forecasts to inform the public about daily air pollution levels and the resultant health impacts in their communities. During FY-2003, the AIRNow program was expanded to include daily forecasts of $PM_{2.5}$ levels in over 100 cities across the United States. To enable forecasts of particle pollution from State/Local air pollution control agencies, ASMD helped develop the EPA guidance document, *Guidelines for Developing an Air Quality* (*Ozone and* $PM_{2.5}$) *Forecasting Program* (U.S. EPA, 2003). Division staff also worked with EPA on several other activities designed to assist State/Local air quality forecasters in issuing accurate $PM_{2.5}$ next-day forecasts. Four training workshops were conducted to inform State and Local forecasters of the latest tools and techniques associated with particle pollution forecasting. A series of statistical and qualitative forecast tools were developed for 22 major metropolitan areas across the United States. Finally, a variety of software products were developed to ease the day-to-day forecast burden. The combination of the AIRNow infrastructure and the NOAA/EPA air quality forecast model is expected to yield even greater amounts of air quality and health impact information.

2.6.2 Support to the NOAA Office of the Federal Coordinator for Meteorology

In December 2001, the Office of the Federal Coordinator for Meteorology (OFCM) hosted the Workshop on Effective Emergency Response Selecting a Suitable Dispersion Model for a Given Application. The participants considered what kinds of models are used in specific situations and how atmospheric transport and diffusion (ATD) modeling systems are evaluated. The goal of the workshop was to define a framework for supporting the objective determination of the most appropriate dispersion modeling system to be used in a given situation. This workshop served as the impetus for the OFCM to lead the Federal ATD modeling community in a concerted effort to evaluate the ATD models available to address typical threats.

In January 2002, OFCM formed the Joint Action Group for Selection and Evaluation of Atmospheric Transport and Diffusion Models (JAG/SEATD) and charged the participants to review the ATD modeling systems in use by the Federal agencies at operational modeling centers and to conduct a preliminary analysis of gaps in understanding, and recommend areas for research and development. The JAG/SEATD met approximately monthly through July 2002, and summarized its findings in a report (Hicks *et al.*, 2002). While there are over 140 documented ATD models used for regulatory purposes, research and development, and emergency operations, the JAG/SEATD narrowed the list to only 29 non-proprietary modeling systems that are used operationally either by first responders and/or at the Federal operational modeling centers. These 29 modeling systems were the focus of the JAG/SEATD's evaluation. The analysis of the gaps in the understanding and capabilities of ATD modeling systems yielded factors that require further research and development. The factors range from source characterization to the study of the effects of complex terrain, coastal influences, and urban areas.

During the summer of 2003, the OFCM assisted Federal agencies having expertise in ATD modeling systems to develop an interagency framework to provide tailored all-hazards assessments for the Department of Homeland Security (DHS). The purpose of the framework is to provide the best available information for atmospheric hazard predictions so that DHS can make appropriate emergency response and consequence management decisions. The framework designates the primary agency to be contacted, and specifies a progression of backup agencies to provide redundancy. A communication protocol would be established so that in an emergency those modeling centers with the appropriate expertise are alerted and a common understanding of the emergency is established. Each contacted agency would provide an initial characterization, which would be updated and refined as new information becomes available. The results from each agency may differ due to differences in the underlying assumptions reflecting the uncertainties of the situation, but summarizing all the results will provide a robust characterization of the overall uncertainty. By this means, the primary agency can provide DHS a tailored assessment of the probable impact of an airborne release and a summary of the uncertainties associated with the assessment. To implement the framework, a common GIS software (*e.g*., GRASS©[5], ArcGIS©™[6]) must be selected that can be used by each agency in expressing its characterization of the impacts and uncertainties. Once this is selected, then the cost of implementing the framework is whatever it takes for each agency to convert its ATD predictions to the common format for dissemination and use.

2.6.3 Sensitivity of $PM_{2.5}$ Modeling to Grid Resolution

As part of an exercise to develop EPA guidance to direct State/Local $PM_{2.5}$ attainment demonstrations, Division staff modeled a series of sensitivity runs using CMAQ to consider the effects of 36-, 12-, 4-km grid cell size on PM control signal and signal strength. The modeling analysis was completed for a limited summer case, July 7–15, 1995, using an older version of the CMAQ model.

The major conclusions from this short-term sensitivity modeling was that control ratios can vary as a function of grid resolution, but the differences are generally small between 36 and 12 km in these simulations (*e.g*., only 21% of the simulated city/control cases show differences of greater than 1%, and only 10% of the cases show differences of greater than 2%). The largest base/control differences are generally seen in cases involving nitrate replacement. For example, the effect of a 25% SO_x cut in Baltimore was a 29% increase in nitrate in the 36 km grid, but only a 18% increase in the 12 km grid. The control ratios in the 4 km grid were generally similar for $PM_{2.5}$, but could vary widely for ozone based on the titration of ozone by NO emissions with the urban core.

2.6.4 Community Modeling and Analysis System Center

FY-2003 was the second year of the cooperative agreement, begun at the initiative of ASMD for the establishment and operation of Community Modeling and Analysis System Center (CMAS) in support of the Models-3/CMAQ air quality modeling system. During FY-2003, the cooperative agreement was transferred from the MCNC North Carolina Supercomputing Center to the Carolina Environmental Program of the University of North Carolina at Chapel Hill (UNC-CH). All CMAS Internet-based support functions were migrated to computers maintained by UNC-CH and are located at www.cmascenter.org. CMAS strengthened its crucial role in the growth and sustenance of the CMAQ user community by providing expanded collaboration in

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[5]GRASS (Geographic Resources Analysis Support System) is Copyright, 1999-2002 by the GRASS Development Team, and licensed under terms of the GNU General Public License.

[6]Copyright to Environmental Systems Research Institute, Inc. (ESRI); ArcGIS is a trademark of ESRI.

model improvements, regularly scheduled training, and support. The CMAS on-line support functions were expanded to include on-line bulletin boards to allow users to share information on specific Models-3/CMAQ topics, in addition to the automated bug-tracking system, users listserv, and Frequently Asked Question section. Internet information and data clearinghouse capabilities were also added to the CMAS web site. CMAS is now the portal for public release of EPA air quality modeling products. The computer code and documentation for CMAS-supported modeling products can be accessed through the CMAS web site. Current products include the Models-3 IO/API, CMAQ, SMOKE©, MIMS, and PAVE©[7] (Package for Analysis and Visualization).

CMAS continued active outreach to the Models-3/CMAQ user community during FY-2003. The Models-3 listserv reflected expanded use of the modeling in products in Europe (England, Germany, Spain, Bulgaria) and Asia (China, Taiwan, Japan), as well as in North America. The First CMAS User's Workshop was held October 21–23, 2002, at the EPA facilities in Research Triangle Park, North Carolina. There were over 110 participants and 40 presentations. At the end of FY-2003, the second workshop was being planned for October 2003, with increased registration and number of presentations expected. CMAS User's Workshop papers and presentations are available at www.cmascenter.org/workshop.shtml.

2.6.5 Particle Deposition—Comparison of Aerodynamic and Mechanical Resuspension Mechanisms

Resuspension of uniform latex microspheres deposited on a single seed pod of field Rye grass stalk and head was investigated experimentally in a wind tunnel. The experiment was designed to answer the following questions:

(1) Does the mechanical disturbance of grass (hereafter abbreviated by "M") increase the resuspension rate of particles deposited on grass when compared to the action of aerodynamic mechanisms (hereafter abbreviated by "A") alone? Examples of A are direct actions of the turbulent air motions: vibration of vegetative surfaces, production of sweeping eddies that may detach particles, and viscous forces that remove particles at the mean wind speeds. The mechanical disturbance (M) considered in this experiment was the striking of the oscillating grass stalk against a stationary object in response to turbulent air motions.

(2) Does particle size affect the particle flux enhancement of the M mechanism?

The experiment was run for water-suspended spherical latex particles with diameters from 2 to 10 µm painted onto seed pods of grass. Wind tunnel tests were run for wind speeds

[7]Copyright 1997-2000 MCNC-North Carolina Supercomputing Center, Research Triangle Park, NC.

from 2 to 18.5 ms^{-1} and a turbulence intensity (root-mean-square fluctuation wind speed /mean wind speed) of 0.1. A locally available rye grass field (Secale Cercele) was chosen.

Experimental results for 2 µm microsphere tests suggest an exponential decrease of resuspension with time. The data show that the flux of 2 µm particles is not sustained for wind tunnel winds less than 12.4 m s^{-1}. Above 12.4 m $s^{-1,}$ the flux is sustained. For wind speeds below 12.4 m s^{-1}, particles are seen coming off the grass for a limited period of time. This is interpreted as a small fraction of the particles being loosely adhering to the grass that are depleted soon following the start of the test. The A threshold of 12.4 m s^{-1} was used based on our data. Likewise the threshold for the A mechanisms for the other particle sizes is given in Table 3.

Table 3. Threshold centerline tunnel speed vs. particle size and ratio of resuspension fluxes for A to (A+M).

Diam, µm	2	3.2	4.5	8.1
Threshold, ms^{-1}	12.4	13.5	13.5	16.7
Ratio of Fluxes A to (A+M), %	15	44	43	47

Ratios of the fluxes for aerodynamic forces only (A) to fluxes for aerodynamic plus mechanical (impacting grass) mechanisms (A + M) were calculated and are given in Table 3. Whereas the resuspension of 2 µm microspheres was dominated by mechanical resuspension, viscous/turbulent resuspension is almost equally effective for 3.2 and 4.5 µm microspheres. However, this ratio is probably underestimated because the tests for A + M resuspension were always done following tests of A resuspension; that is, mechanical resuspension always operated on an already depleted particle source. For 8.1 µm microspheres, the table shows that the thresholds for A resuspension were at the upper part of the range of our wind tunnel speeds; the A and M resuspension mechanisms were not fully developed at our highest wind tunnel speeds compared to the 2, 3.2, and 4.5 µm microspheres.

The findings from these experiments suggest the following: (1) Resuspension particle flux increases when mechanical impacts occur; and (2) mechanical resuspension dominates for 2 µm particles over purely aerodynamic resuspension, but for larger particles aerodynamic mechanisms are roughly equally effective in resuspending particles.

2.6.6 NARSTO Program Support

NARSTO, a multi-stakeholder entity, was organized in 1994 to sponsor cooperative, public/private, policy relevant research on tropospheric ozone. In 1999, NARSTO's charge was expanded to include airborne particulate matter. Currently, its research programs focus on both ozone and PM, including their combined atmospheric chemistry and physics. As a major part of its charter, periodic policy relevant science assessments are commissioned. Its first assessment was the 2000 Ozone Assessment and the second was the February 2003 Particulate Matter Science Assessment.

NARSTO is an umbrella organization with a bottom-up management structure where each member controls its own resources, but contributes to a larger cause. NARSTO activities in the PM arena fall into two general categories: direct NARSTO efforts, and internal efforts conducted by NARSTO member organizations. Items in the first category are easy to list, while those in the second are more difficult. A number of NARSTO's collective efforts, particularly the field studies, deal with gaseous pollutants as well as particles.

Direct NARSTO efforts:

- Production of the NARSTO PM Assessment
- Archival of the PM Super-Site data in the NARSTO data archive
- Organization and conduct of the NARSTO Workshop on Advanced Techniques for Emission-Inventory Development and Verification (Austin, TX, October 2003)
- Organization and conduct of the meeting: Tropospheric Aerosols: Science and Decisions in an International Community (Querétaro, Mexico, October 2000)

Collective NARSTO efforts:

- California Regional Particulate Air Quality Study (2000, San Joaquin Valley)
- Texas 2000 Field Study (East Texas)
- Pacific 2001 Field Study (Southwestern Canada)
- PNW 2001 Field Study (Northwestern United States)
- Mexico City Metropolitan Area 2003 Field Campaign

Individual NARSTO members contribute significantly to the advancement of the understanding of atmospheric chemistry and physics, measurement technique development, computer modeling, and emission characterization. More information can be found at:
http://www.cgenv.com/Narsto/

2.6.7 European Monitoring and Evaluation Program

A Division scientist serves as the United States representative to the European Monitoring and Evaluation Program (EMEP) that oversees the cooperative program for monitoring and evaluation of the long-range transmission of air pollutants in Europe. The primary goal of EMEP is to use regional air quality models to produce assessments evaluating the influence of one country's emissions on another country's air concentrations or deposition. The emphasis has shifted from acidic deposition to ozone and there is now interest in fine particulates and toxic chemicals. The United States and Canadian representatives report on North American activities related to long-range transport. The Division scientist also evaluates

European studies of special relevance to the program, providing technical critiques of the EMEP work during formal and informal interactions, and develops and coordinates such programs with EMEP as the modeling studies of the Modeling Synthesizing Center West at the Norwegian Meteorological Institute in Oslo, Norway. In FY-2002, the United States and Canadian representatives offered to host a workshop on fine particulate matter measurement and modeling to summarize the experiences of the EPA Supersite program for the benefit of the EMEP program. The offer was enthusiastically accepted by EMEP. The workshop will be held in April 2004 in New Orleans, Louisiana.

2.6.8 Modeling Human Exposure to Solar Ultraviolet Light Modeling Human Exposure to Solar Ultraviolet Light

Solar ultraviolet radiation is a known human carcinogen and a causal agent in cataract induction. Experimental exposure assessment methods are currently limited to mannequin studies or human volunteers performing scripted scenarios wearing UV-sensitive polysulfone film badges. The modeling approach presented will enable calculation of the relative distribution of sunlight exposure across the anatomy with unprecedented precision, providing dose estimates used in the development of dose/response functions. The model will also be used to quantify continuous duration acute human exposures and compare with controlled laboratory doses known to induce basal cell and melanoma skin cancers in animals. An article will be published describing a simulation model that calculates instantaneous irradiance or cumulative intercepted energy at 40 anatomical locations for an arbitrary sun exposure scenario defined by latitude, longitude, date, time, atmospheric transmissivity, and subject posture.

2.7 Regulatory Support

2.7.1 Ozone Modeling Completed in Support of the Interstate Transport Rule

Section 110(a)2(d) of the Clean Air Act (CAA) gives EPA the authority to require States to develop plans to prohibit sources from emitting pollutants in amounts that will contribute significantly to nonattainment in any other State. EPA can set emission budgets designed to avoid significant amounts of interstate transport. In support of a proposed rulemaking designed to reduce ozone and $PM_{2.5}$ nonattainment in the future, Division staff completed an air quality modeling analysis to consider whether significant State-to-State ozone transport affecting 8-hour ozone nonattainment areas will exist in 2010.

The Comprehensive Air Quality Model with Extensions (CAMx) was used to assess 8-hour ozone concentrations as part of this proposed rulemaking. CAMx is a publicly available Eulerian model that accounts for the processes that are involved in the production, transport, and destruction of ozone over a specified three-dimensional domain and time period. The model simulations were performed for a domain covering the eastern United States and adjacent portions of Canada. Three episodes during the summer of 1995 were used for modeling ozone and precursor pollutants: June 12–24, July 5–15, and August 10–21. An operational evaluation was completed, which concluded that, on average, the model-predicted patterns and day-to-day variations in regional ozone levels are similar to what was observed with measured data. Ozone modeling was performed using 2001 emissions and for 2010 and 2015 base cases as part of the approach for forecasting which counties are expected to be in nonattainment in these two future years. In general, the approach involved using the model in a relative sense to estimate the change in ozone between 2001 and each future base case.

The modeling approach used by EPA to quantify the downwind impact of emissions in specific upwind States to projected downwind nonattainment for 8-hour ozone included two different techniques, zero-out and source apportionment. The outputs of the two modeling techniques were used to calculate metrics or measures of contribution. The metrics were evaluated, for each State/State linkage, to determine which States make a significant air quality contribution to downwind ozone nonattainment in other States. These two techniques provided different technical approaches to quantifying the downwind impact of emissions in upwind States. The zero-out modeling analysis provided an estimate of downwind impacts by comparing the model predictions from a base case run to the predictions from a run in which the base case man made emissions were removed from a specific State. In contrast to the zero-out approach, the source apportionment modeling quantified downwind impacts by tracking the impacts of ozone formed from emissions in an upwind source area. The EPA selected several metrics to quantify the projected downwind contributions from emissions in upwind States. The metrics were designed to provide information on three fundamental factors for evaluating whether emissions in an upwind State make large and/or frequent contributions to downwind nonattainment. These factors are: a) the magnitude of the contribution, b) the frequency of the contribution, and c) the relative amount of the contribution. The magnitude of contribution factor refers to the actual amount of ozone contributed by emissions in the upwind State to nonattainment in the downwind area. The frequency of the contribution refers to how often contributions above certain thresholds occur. The relative amount of the contribution is used to compare the total ozone contributed by the upwind State to the total amount of nonattainment ozone in the downwind area. The factors are the basis for several metrics that can be used to assess the significance of a particular impact. The metrics used in this analysis were the same as those used in the NO_x SIP Call. The findings of this modeling analyses were that significant ozone transport is likely to exist over broad portions of the eastern United States by 2010.

2.7.2 Air Quality Modeling Completed in Support of the 8-Hour Ozone Implementation Rule

In June 2003, EPA proposed a rule to implement the 8-hour ozone NAAQS. As part of the background information for the rulemaking, an economic analysis of the costs and benefits of the 8-hour ozone NAAQS was initiated. To guide this cost-benefit analysis, a series of 34 CAMx modeling runs were completed to assess the emission reductions necessary to meet the air quality standard by the attainment dates outlined in the rule. Each of the CAMx simulations considered differing levels of NO_x versus VOC control and various combinations of regional versus local controls. Attainment targets were estimated for areas projected to be in nonattainment of the 8-hour ozone NAAQS.

As an example, the analysis indicated that the Providence, Rhode Island, metropolitan statistical area would need either a) an additional 15% reduction in local NO_x emissions, b) an additional 10% reduction in local NO_x plus VOC emissions, or c) an additional 10% reduction in local NO_x emissions in conjunction with a reduction in regional NO_x emissions. These results were input into an EPA economic model to determine the least cost set of controls that would yield attainment. In general, the modeling concluded that large amounts of additional ozone precursor control, beyond already promulgated measures, would be needed for several metropolitan areas in the eastern United States to reach attainment by 2007, 2010, and/or 2013.

2.7.3 Ozone Modeling Completed in Support of the Nonroad Rule

In May 2003, EPA proposed to reduce emissions from nonroad diesel engines as a means of reducing the population exposed to nonattainment levels of ozone and $PM_{2.5}$. To demonstrate the need for, and the impact of the rule, ASMD performed CAMx modeling simulations of two separate 36 and 12 km resolution domains, one covering the eastern United States and the other covering the western United States. For the eastern United States domain, the model was applied and evaluated over three episodes that occurred during the summer of 1995 base year. For the western United States, two episodes that occurred during the summer of 1996 were modeled using base year emissions. Subsequently, episodic ozone model runs were made for 2020 and 2030 base and control case scenarios for both domains and all episodes.

The model outputs from the 1996 base year and 2020 and 2030 base cases, combined with current air quality data, were used to identify areas expected to exceed the ozone NAAQS in 2020 and 2030. These projected nonattainment areas will require additional emission reductions to attain and maintain the ozone NAAQS. The costs, benefits, and expected impacts of the proposed controls were determined by comparing the model results in the future year control runs against the baseline simulations of the same year. Ultimately, the modeling supported the conclusions that there would potentially be several metropolitan areas with predicted ozone concentrations at or above the NAAQS in the 2020 and 2030 base case scenarios without additional emission reductions; and that the proposed nonroad emissions reductions could be expected to substantially improve ozone levels in the future.

2.7.4 Sensitivity Modeling Analyses for Regulatory Applications of CMAQ

ASMD conducted several model diagnostic tests to assess the status of the CMAQ model and its suitability for regulatory support modeling. The results of some of these analyses were used to support model developmental work. The effect of alternative roughness lengths and their seasonality in MCIP were assessed. A series of runs investigating the effect of using pass-thru options in MCIP versus recalculating PBL heights and radiation fields were completed. The

Division also assessed the effect of using revised versions of MCIP (v2.1 and v2.2). The sensitivity of the model to the minimum Kv (Kv=Vertical diffusion coefficent) value within CMAQ was considered, as was the effects of changes in CMAQ deposition velocities. Finally, modeling was conducted to assess the effects of revisions to CMAQ horizontal diffusivities.

2.7.5 Meteorological Classification to Augment Speciated Pollution Data

A plan was developed to use meteorological data to assess seasonal speciation data to determine source locations of high particulate matter (PM). Hourly meteorological data was gathered for many sites within the United States by the NOAA. These sites tend to be in or near metropolitan areas. An entire year of data is stored on a CD and part of the year 2001 and 2002 was used. Meteorological data from September 2001 through November 2001 will be used for the fall season, December 2001 through February 2002 for the winter season, March through May 2002 for the spring season, and June through August 2002 for the summer season.

Meteorological data is being downloaded to a spreadsheet for 45 urban stations throughout the United States. The meteorological data to be used include temperature, wind direction and speed, relative humidity, and rainfall will be averaged over each of the four seasons described above. This data will then be used to assess the speciated PM data that was collected over the same time periods.

2.7.6 Support Center for Regulatory Air Models

SCRAM (Support Center for Regulatory Air Models) website continued to be updated to reflect addition of models and data sets, including modifications to AERMOD deposition; these updates comply with the official EPA web page template, as directed by the Office of Environmental Information, and with EPA OAQPS guidelines for regulatory air models. Additional references and links were created to provide easier maneuvering to specific models and related files. Updates also related to the *7th Modeling Conference for Air Quality Modeling* (http://www.epa.gov/scram001/tt26.htm) were made. SCRAM serves as the sole Internet source for the EPA's air quality dispersion models, guidance, and related programs and information.

REFERENCES

American Society for Testing and Materials. *Standard Guide for Statistical Evaluation of Atmospheric Dispersion Model Performance* (D 6589). West Conshohocken, PA 19428, 17 pp. (2000). Available at http://www.astm.org.

Arnold, J.R., R.L. Dennis, and G.S. Tonnesen. Diagnostic evaluation of numerical air quality models with specialized ambient observations: Testing the Community Multiscale Air Quality (CMAQ) modeling system at selected SOS 95 ground sites. *Atmospheric Environment* 37:1185–1198 (2003).

Barad, M.L. (Ed.). Project Prairie Grass, a Field Program in Diffusion. Geophysical Research Papers, No. 59, Vols. I and II. Air Force Cambridge Research Center Report AFCRC-TR-58-235, 479 pp. [NTIS PB 151 425 and PB 151 424] (1958).

Bowne, N.E., R.J. Londergan, D.R. Murray, and H.S Borenstein. Overview, results, and conclusions for the EPRI plume model validation and development project: Plains site. EPRI EA-3074, Project 1616-1, Electric Power Research Institute, Palo Alto, CA, 234 pp. (1983).

Brown, M. Urban parameterizations for mesoscale meteorological models. In *Mesoscale Atmospheric Dispersion*. Z Boybeyi (Ed.). WIT Press, Boston, 424 pp. (2000).

Ching, J., A. Lacser, T. Otte, and S. Dupont. Air quality simulations at neighborhood scales with CMAQ. *Proceedings of the 4th International Conference on Urban Air Quality—Measuring, Modeling and Measurement, Charles University, Prague, Czech Republic, March 25-28, 2003*. Institute of Physics, the Charles University, and the University of Hertfordshire in collaboration with SATURN and COST715, Charles University, Prague, CZ, 47–50 (2003).

Cohn, R.D., B.K. Eder, S.K. LeDuc, and R.L. Dennis. Development of an aggregation and episode selection scheme to support the Models3 Community Multiscale Air Quality Model. Journal of Applied Meteorology 40:210–228 (2001).

Cohen, Y., and E.J. Cooter. Multimedia environmental distribution of toxics (Mend-Tox): Part I, Hybrid compartmental-spatial modeling framework. *Practice Periodical Hazardous, Toxic, and Radioactive Waste Management* 6:70–86 (2002a).

Cohen, Y., and E.J. Cooter. Multimedia environmental distribution of toxics (Mend-Tox): Part II, Software implementation and case studies. *Practice Periodical Hazardous, Toxic, and Radioactive Waste Management* 6:87–101 (2002b).

Dennis, R.L., J.R. Arnold, and G.S. Tonnesen. On the need for better ambient observations of important chemical species for air quality model evaluation. W.A. McClenny (Ed.). In

Recommended methods for ambient air monitoring of NO, NO_2, NY_Y, and individual NO_Z species. EPA/600/R-01/005, National Exposure Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC, 8–21 (2001).

Dupont, S., T.L. Otte, and J. S. Ching. Simulation of the meteorological fields within and above urban and rural canopies with a mesoscale model (MM5). *Boundary-Layer Meteorology* (accepted for publication)(a).

Dupont, S., I. Calmet, P. Mestayer, and S. Leroyer. Parameter**isa**tion of the urban energy budget with the SM2-U model for the urban boundary layer simulation. *Boundary-Layer Meteorology* (accepted for publication)(b).

Gego, E., C. Hogrefe, G. Kallos, A. Voudouri, P.S. Porter, J.S. Irwin, and S.T. Rao. Examination of model predictions at different horizontal grid resolutions. *Environmental Fluid Mechanics* (accepted for publication)(a).

Gego, E., P.S. Porter, J. Irwin, C. Hogrefe and S.T. Rao. Assessing the comparability of ammonium, nitrate and sulfate concentrations measured by three air quality monitoring networks. *Pure and Applied Geophysics* (Accepted for publication)(b).

Gillani, N.V., and J.M. Godowitch. Plume-in-grid treatment of major point source emissions. In *Science algorithms of the EPA Models-3 Community Multiscale Air Quality modeling system*. Chapter 9. D.W. Byun, and J.K.S. Ching (Eds.). EPA-600/R-99/030, National Exposure Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC, 1–40 (1999).

Gilliland, A.B., R.L. Dennis, S. Roselle, and T. Pierce. Seasonal NH_3 emission estimates for the eastern United States based on wet ammonium concentrations and an inverse modeling method. *Journal of Geographical Research-Atmospheres*108(D15), 4477, doi:10.1029/2002JD003063 (2003).

Godowitch, J.M. Photochemical and aerosol modeling with the CMAQ plume-in-grid approach. *Preprints, 12th Joint Conference on the Applications of Air Pollution Meteorology with A&WMA, May 20–24, 2002, Norfolk, Virginia.* American Meteorological Society, Boston, 69–70 (2002).

Haugen, D.A. (Ed.). Project Prairie Grass, a Field Program in Diffusion. Geophysical Research Papers. No. 59, Vol. III. Air Force Cambridge Research Center Report AFCRC-TR-58-235, 673 pp. [NTIS PB 161 101] (1959).

Hertel O., R. Berkowicz, J. Christensen, and O. Hov. Test of two numerical schemes for use in atmospheric transport-chemistry models. *Atmospheric Environment* 27A:2591-2611 (1993).

Hicks, B., R. Addis, W. Bach, T. Bauer, B. Beitler, P. Davidson, J. Ellis, D. Garvey, J. Irwin, J. Mitchell, D. Payton, D. Randerson, and J. Sarkisian. *Atmospheric Modeling for Releases from Weapons of Mass Destruction: Response by Federal Agencies in Support of Homeland Security*. FCM-R17-2002. August, 2002, U.S. Department of Commerce, Office of the Federal Coordinator for Meteorological Services and Supporting Research, Silver Spring, MD, 160 pp. (2002).

Holben, B.N., T. Eck, I Slutsker, D. Tanre. AERONET—A federated instrument network and data archive for aerosol characterization. *Remote Sensing of the Environment* 66:1–16 (1998).

Irwin, J., D. Carruthers, J. Paumier, and J. Stocker. Application of ASTM D6589 to evaluate dispersion model performance. *International Journal of Environment and Pollution*. 20(1–6):4–10 (2003).

Jacob, D.J. Heterogenous chemistry and tropospheric ozone. *Atmospheric Environment* 34:2131–2159 (2000).

Kahn, R., P. Banerjee, D. McDonald, and J. Martonchik. Aerosol properties derived from aircraft multiangle imaging over Monterey Bay. *Journal of Geophysical Research-Atmospheres* 106(D11):11977–11995 (2001).

Lacser, A., and T.L. Otte. Implementation of an urban canopy parameterization in MM5. *Preprints, 4th Symposium of Urban Environment, May 20-24, 2002, Norfolk, Virginia*. American Meteorological Society, Boston, 153–154 (2002).

Martelli, A., A. Clappier, and M. Rotach, 2002: An urban surface exchange parameterizations for mesoscale models. *Boundary-Layer Meteorology* 104(2):261–304 (2002).

Mathur, R., and R.L. Dennis. Seasonal and annual modeling of reduced nitrogen compounds over the Eastern United States: Emissions, ambient levels and deposition amounts. *Journal of Geophysical Research-Atmospheres* 108(D15), 4481 doi:10.1029.2002JD002794 (2003).

Murphy, A.H., B.G. Brown, and Y.-S. Chen. Diagnostic verification of temperature forecasts. *Weather and Forecasting* 4:485–501 (1989).

Murray, D.R., and N.E. Bowne. Urban power plant plume studies. EPRI Report No. EA-5468, Research Project 2736-1, Electric Power Research Institute, Palo Alto, CA (1988).

Olesen, H.R. A platform for model evaluation. *International Journal of Environment and Pollution* 16(1–6):129–136 (2001).

Otte, T.L., and A. Lacser. Implementation of an urban canopy parameterization for fine-scale simulations. *Preprints, Twelfth PSU/NCAR Mesoscale Model Users' Workshop, June 24-25, 2002, Boulder, Colorado*. National Center for Atmospheric Research, Boulder, Colorado 138–140 (2002).

Otte, T.L., A. Lacser, S. Dupont, and J.K.S. Ching. Implementation of an urban canopy parameterization in a mesoscale meteorological model. *Journal of Applied Meteorology* (Accepted for publication).

Pierce, T., W. Benjey, J. Ching, D. Gillette, A. Gilliland, S. He, M. Mebust, and G. Pouliot. Advances in emissions modeling of airborne substances. *Emission Inventories — Applying New Technologies, 12th International Emission Inventory Conference, April 29–May 1, 2003, San Diego, California*. Session 3 — Data Management. Office of Air Quality Planning and Standards, Research Triangle Park, NC, (2003). Available at http://www.epa.gov/ttn/chief/conference/ei12/index.html#ses-9

Pleim, J.E., and A. Xiu. Development of a land surface model. Part II: Data assimilation. *Journal of Applied Meteorology* 42:1811–1822 (2003).

Riemer, N., H. Vogel, B. Vogel, B. Schell, I. Ackermann, C. Kessler, and H. Hass. Impact of the heterogeneous hydrolysis of N_2O_5 on chemistry and nitrate aerosol formation in the lower troposphere under photosmog conditions. *Journal of Geophysical Research-Atmospheres* 108(D4), 4144, doi:10.1029/2002JD002436 (2003).

Sullivan, T.J., B.J. Cosby, J.A Laurence, R.L. Dennis, K. Savig, J.R. Webb, A.J. Bulger, M Scruggs, C. Gordon, J. Ray, E.H. Lee, W.E. Hogsett, H. Wayne, D. Miller, and J.S. Kern. *Assessment of Air Quality and Related Values in Shenandoah National Park*, Technical Report NPS/NERCHAL/NRTR-03/090, National Park Service, U.S. Department of the Interior, Northeast Region, Philadelphia, Pennsylvania (2003).

Taylor, K.E. Summarizing multiple aspects of model performance in a single diagram. *Journal of Geophysical Research-Atmospheres* 106(D7):7183–7192 (2001).

Tonnesen, G.S., and R.L. Dennis. Analysis of radical propagation efficiency to assess ozone sensitivity to hydrocarbons and NO_X. Part 1: Local indicators of instantaneous odd oxygen production sensitivity. *Journal of Geophysical Research - Atmospheres* 105(D7):9213-9225 (2000a).

Tonnesen, G.S., and R.L. Dennis. Analysis of radical propagation efficiency to assess ozone sensitivity to hydrocarbons and NO_X. Part 2: Long-lived species as indicators of ozone concentration sensitivity. *Journal of Geophysical Research-Atmospheres* 105(D7):9227–9241 (2000b).

U.S. Environmental Protection Agency. *Guidelines for developing an air quality (ozone and $PM_{2.5}$) forecasting program*. EPA-456/R-03-002, Office of Air Quality Planning and Standards, Office of Air and Radiation, Research Triangle Park, NC, 96 pp. (2003).

Wu, Y., B. Brashers, P.L. Finkelstein, and J. E. Pleim. A multilayer biochemical dry deposition model, Part 1: Model formulation. *Journal of Geophysical Research-Atmospheres* 108(D1), 4013, doi:10.1029/2002JD002293 (2003a).

Wu, Y., B. Brashers, P.L. Finkelstein, and J.E. Pleim. A multilayer biochemical dry deposition model, Part 2: Model evaluation. *Journal of Geophysical Research-Atmospheres* 108(D1), 4014, doi:10.1029/2002JD002306 (2003b).

Xiu, A., and J. E. Pleim. Development of a land surface model. Part I: Application in a mesoscale meteorology model. *Journal of Applied Meteorology* 40:192–209 (2001).

APPENDIX A: ACRONYMS, ABBREVIATIONS, AND DEFINITIONS

ACM	Asymmetric Convective Model
ADMS	Air Dispersion Modeling System
AE3	Aerosols component version 3
AERMET	AERMOD Meteorological Preprocessor
AERMIC	American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee
AERMOD	AMS/EPA Regulatory Model
AERSCREEN	AERMOD screening model
ArcGIS	A commercial GIS software package
ARL	Air Resources Laboratory
ASMD	Atmospheric Sciences Modeling Division
ASPEN	Assessment System for Population Exposure Nationwide
ASTM	American Society for Testing and Materials
ATD	Atmospheric Transport and Diffusion
ATDD	Atmospheric Turbulence and Diffusion Division, NOAA
AVHRR	Advanced Very High Resolution Radiometer
AVIRIS	Airborne Visible and InfraRed Imaging Spectrometer
BCON	Boundary Concentrations
BEIS-3	Biogenic Emissions Inventory System version 3
BELD	Biogenic Emissions Land cover Database
BELD-3	Biogenic Emissions Land cover Database version 3
BRACE	Bay Regional Atmospheric Chemistry Experiment
CAA	Clean Air Act
CAAA	Clean Air Act Amendments
CALMET-CALPUFF	A diagnostic meteorological model/puff dispersion model
CAMx	Comprehensive Air Quality Model with extensions
CASTNet	Clean Air Status and Trend Network
CB-IV	Carbon Bond version 4
CCM	Community Climate Model
CDOM	Colored, Dissolved Organic Matter
CIRA	Cooperative Institute for Research in the Atmosphere
CMAQ	Community Multiscale Air Quality modeling system
CMAQ-Hg	Community Multiscale Air Quality modeling system mercury model
CMAS	Community Modeling and Analysis System
CONSUME	A fuel consumption model, which predicts total smoldering fuel consumption during wild fires.
CSEM	Community Smoke Emission Model
CTM	Chemistry-Transport Model
DHS	Department of Homeland Security

DOE	Department of Energy
EDAS	Eta Data Assimilation System
EMEP	European Monitoring and Evaluation Program
EPA	Environmental Protection Agency
EPA	Environmental Protection Agency
ESCOMPTE	A European sponsored intensive field study program
Eta	National Center for Environmental Prediction Mesoscale Model
Extended RADM	Regional Acid Deposition Model with full dynamics of secondary inorganic fine particle formation taken from the RPM
FDDA	Four-Dimensional Data Assimilation
GCM	Global Climate Models
GCRP	Global Change Research Program
GCTM	Global Chemical Transport Model
GIS	Geographic Information System
GIS	Graphical Information Software
GISS	Goddard Institute for Space Studies
GRASS	A commercial GIS software package
GRIB	GRIdded Binary files
HAP	Hazardous Air Pollutant
HPDM	Hybrid Plume Dispersion Model
HYSPLIT4	Hybrid Single-Particle Lagrangian Integrated Trajectory model
ICON	Initial Concentrations
IMPROVE	Interagency Monitoring of PROtected Visual Environment Network
ISCST	Industrial Source Complex Model (Short-Term)
ISORROPIA	A computationally efficient thermodynamic model
JAG/SEATD	Joint Action Group for Selection and Evaluation of Atmospheric Transport and Diffusion Models
LADCO	Lake Michigan Air Directors Consortium
LESchem	Large-eddy simulation with the chemistry model
LSODE	Livermore Solver for Ordinary Differential Equation
M3DRY	Models-3 Dry Deposition Scheme
MARAMA	Mid-Atlantic Regional Air Management Association
MCIP	Meteorology-Chemistry Interface Processor
MCIP2	Meteorology-Chemistry Interface Processor version 2
MDN	Mercury Deposition Network
MEBI	Modified Euler Backward Iterative
MEND-TOX	Multimedia Environmental Distribution of TOXics
MIC3	Meteorological Instrumentation Cluster of 3
MIMS	Multimedia Integrated Modeling System
MM5	Mesoscale Model - version 5
Mobile6	Mobile Source Emission Model

MODTRAN	MODerate resolution radiative TRANsfer model
MOVES	Multiscale mOtor Vehicle and equipment Emission System
MPRM	Meteorological Preprocessor for Regulatory Modeling
NAAQS	National Ambient Air Quality Standards
NALCC	North American Land Cover Characteristics
NASA	National Aeronautics and Space Administration
NATA	National Air Toxics Assessment
NCAR	National Center for Atmospheric Research
NEI	National Emission Inventory
NERL	National Exposure Research Laboratory
NHEERL	National Health and Environmental Effects Research Laboratory
NLCD	National Land Cover Database
NMSE	Normalized Mean Square Error
NOAA	National Oceanic and Atmospheric Administration
NO_x	Nitrogen oxides
NPS	National Park Service
NRMRL	National Risk Management Research Laboratory
NSR	New Source Review
NWS	National Weather Service
OBMs	Observations-Based Methods
ODE	Ordinary Differential Equation
OFCM	Office of the Federal Coordinator for Meteorology
OTAQ	EPA Office of Transportation and Air Quality
PBL	Planetary Boundary Layer
PCDD's	Poly-Chlorinated Dibenzo-p-Dioxins
PCDF's	Poly-Chlorinated Dibenzo-Furans
PCM	Parallel Climate Model
PDE	Partial Differential Equation
PDFs	Probability Density Functions
PDM	Plume Dynamics Model
PinG	Plume-in-Grid
PinG Module	Plume-in-Grid Model
PM	Particulate Matter
PNNL	Pacific Northwest National Laboratory
PX LSM	Pleim Xiu Land-Surface Model
QSSA	Quasi-Steady State Approximation
RADM2	Regional Acid Deposition Model version 2
RAMS	Regional Atmospheric Modeling System
RFA	Request for Assistance
RPCA	Rotated Principal Component Analysis
RPM	Regional Particulate Model
SAPRC99	A gas-phase chemical mechanism

SCRAM	Support Center for Regulatory Air Models
SM2-U	An urban soil model
SMOKE	Sparse Matrix Operator Kernel Emission model
SOA	Secondary Organic Aerosol
SOS	Southern Oxidants Study
STN	Speciation and Trend Network
SWMM	Storm Water Management Model
TexAQS	Texas Air Quality Study of Houston
TKE	Turbulent Kinetic Energy
TMDL	Total Maximum Daily Loan
TTCP-CBD	The Technical Cooperation Program (TTCP) Chemical, Biological and Radiological Defense (CBD)
UAM-V	Urban Airshed Model (Variable Grid)
UCPs	Urban Canopy Parameterizations
USFS	U.S. Forest Service
USGS	U.S. Geological Survey
VOC	Volatile Organic Compounds
WRF	Weather Research and Forecast
WTC	World Trade Center

APPENDIX B: PUBLICATIONS

Arnold, J.R., R.L. Dennis, and G.S. Tonnesen. Diagnostic evaluation of numerical air quality models with specialized ambient observations: Testing the Community Multiscale Air Quality (CMAQ) modeling system at selected SOS 95 ground sites. *Atmospheric Environment* 37:1185–1198 (2003).

Athanassiadis, G.A., S.T. Rao, J.Y. Ku, and R.D. Clark. Boundary layer evolution and its influence on ground-level ozone concentrations. *Environmental Fluid Mechanics* 2:339–357 (2003).

Athanassiadis, G.A., and S.T. Rao. Spatial and temporal variations in the trace elemental data over the northeastern United States. *Environmental Pollution* 123:439–449 (2003).

Benjey, W.G., E. Cooter, A. Gilliland, A.E. Grambsch, E.L. Wright, C.D. Geron, C. Gage, and D.A. Winner. Creating an emission inventory for modeling global climate change effects on regional air quality. In *The Twelfth International Emission Inventory Conference: Applying New Technologies, San Diego, California, April 29-May 1, 2003.* Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, NC, (2003). Available at http://www.epa.gov/ttn/chief/conference/ei12/index.html#ses-10

Binkowski, F.S., and S.J. Roselle. Models-3 Community Multiscale Air Quality (CMAQ) model aerosol component 1. Model description. *Journal of Geophysical Research-Atmospheres* 108(D6), 4183, doi:10.1029/2001JD001409 (2003).

Brankov, E., R.F. Henry, K.L. Civerolo, W. Hao, S.T. Rao, P.K. Misra, R. Bloxam, and N. Reid. Assessing the effects of transboundary pollution between Ontario, Canada and New York, USA. *Environmental Pollution* 123:403–411 (2003).

Ching, J., A. Lacser, T. Otte, and S. Dupont. Air quality simulations at neighborhood scales with CMAQ. *Proceedings of the 4th International Conference on Urban Air Quality: Measuring, Modeling and Measurement, Charles University, Prague, Czech Republic, March 25-28, 2003*. Institute of Physics, the Charles University, and the University of Hertfordshire in collaboration with SATURN and COST715 and supported by AWMA and IUAPPA, 47–50 (2003).

Civerolo, K.L., E. Brankov, S.T. Rao, K. Roy, G.P. Lewis, and P. Galvin. Analysis of ambient, precipitation-weighted, and lake sulfur concentrations in the Adirondack Region of New York. *Environmental Pollution* 123:337–345 (2003).

Civerolo, K., H. Mao, and S.T. Rao. The airshed for ozone and fine particulate pollution in the eastern United States. *Pure and Applied Geophysics* 160:81–105 (2003).

Cooter, E., W. Hutzell, W. Foreman, and M. Majewski. A regional atmospheric fate and transport model for atrazine 2 Evaluation. Environmental Science & Technology 36(21) 4593-4599 (2002).

Dupont, S., T. Otte, A. Lacser, and J. Ching: Using MM5 to simulation the meteorological fields at neighborhood scales. *Proceedings of the 4th International Conference on Urban Air Quality: Measuring, Modeling and Measurement, Charles University, Prague, Czech Republic, March 25-28, 2003.* Institute of Physics, the Charles University, and the University of Hertfordshire in collaboration with SATURN and COST715 and supported by AWMA and IUAPPA, 428-431 (2003).

Gego, E., C. Hogrefe, S. T. Rao, and P. S. Porter. Probabilistic assessment of regional scale ozone pollution in the eastern United States. In, *Air Pollution in Regional Scale. Proceedings of the NATO Advanced Research Workshop, Kallithea, Halkidiki, Greece, June 13–15, 2003.* NATO Science Series: IV. Earth and Environmental Sciences. D. Melas, and D. Syrakov (Eds.). Kluwer Academic Publishers, 87–96 (2003).

Gilliland, A.B., T.J. Butler, and G.E Likens. Monthly and annual bias in weekly (NADP/NTN) versus daily (AIRMoN) precipitation chemistry data in the eastern USA. *Atmospheric Environment* 36:5197–5206 (2002).

Gilliland, A.B., R.L. Dennis, S.J. Roselle, and T.E. Pierce. Seasonal NH_3 emission estimates for the eastern United States based on ammonium wet concentrations and an inverse modeling method. *Journal of Geophysical Research-Atmospheres* 108(D15), 4477, doi:10.1029/2002JD003063 (2003).

Hogrefe, C., S. Vempaty, S.T. Rao, and P.S. Porter. A comparison of four techniques for separating different time scales in atmospheric variables. *Atmospheric Environment* 37:313–325 (2003).

Kang, D., B. Eder, and K. Schere. The evaluation of regional-scale air quality models as part of NOAA's air quality forecasting pilot program. *Proceedings of the 26th NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Applications, Istanbul, Turkey, May 26–30, 2003.* NATO/CCMS International Technical Meeting of Air Pollution Modeling and Its Applications, 404–411 (2003).

Liu, G., C. Hogrefe, and S.T. Rao. Evaluating the performance of regional-scale meteorological models: Effect of clouds simulation on temperature prediction. *Atmospheric Environment* 37:1425–1433 (2003).

Mathur, R., and R.L. Dennis. Seasonal and annual modeling of reduced nitrogen compounds over the eastern United States: Emissions, ambient levels, and deposition amounts. *Journal of Geophysical Research-Atmospheres* 108(D15), 4481, doi:10.1029/2002JD002794 (2003).

Mebust, M. R., B.K. Eder, F.S. Binkowski, and S.J. Roselle. Models-3 Community Multiscale Air Quality (CMAQ) model aerosol component - 2. Model evaluation. *Journal of Geophysical Research,* 108(D6), 4184, doi:10.1029/2001JD001410, (2003).

Mihailovic, D.T., S.T. Rao, C. Hogrefe, and R.D. Clark. An approach for the aggregation of aerodynamic surface parameters in calculating the turbulent fluxes over heterogeneous surfaces in atmospheric models. *Environmental Fluid Mechanics* 2(4):315–337 (2003).

Minville, F., B. Marticorena, D.A. Gillette, R.E. Lawson, R. Thompson, and G. Bergametti. Relationship between the aerodynamic roughness length and roughness density for low roughness density. *Environmental Fluid Mechanics* 3: 269–273 (2003).

NARSTO. *Particulate Matter Science for Policy Makers—A NARSTO Assessment. Parts 1 and 2*. NARSTO Management Office (Envair), Pasco, Washington. (2003). http://www.cgenv.com/Narsto/.

New York State Department of Environmental Conservation. *Assessing the effects of transboundary pollution on New York's Air Quality*. S.T. Rao (Principal Investigator). NYSERDA Final Report 03-02 (2003).

New York State Department of Environmental Conservation. *Analysis of ozone and fine particulate matter in the northeastern United States*. S.T. Rao (Principal Investigator). NYSERDA Final Report 03-04 (2003).

Pastor, S.H., J.O. Allen, L.S. Hughes, P. Bhave, G.R. Cass, and K.A. Prather. Ambient single particle analysis in Riverside, California, by aerosol time-of-flight mass spectrometry during the SCOS97-NARSTO. *Atmospheric Environment* 37:S239–S258 (2003).

Pierce, T., W.G. Benjey, J. Ching, D. Gillette, A. Gilliland, S. He, M. Mebust, and G. Pouliot. Advances in emission modeling of airborne substances. In *The Twelfth International Emission Inventory Conference: Applying New Technologies, San Diego, California, April 29–May 1, 2003*. Office of Air Quality Planning and Standards. U.S. Environmental Protection Agency, Research Triangle Park, NC (2003). Available online at http://www.epa.gov/ttn/chief/conference/ei12/index.html#ses-10

Pouliot, G., and T. Pierce. Emissions processing for an air quality forecasting model. In *The Twelfth International Emission Inventory Conference: Applying New Technologies, San Diego, California, April 29–May 1, 2003*. Office of Air Quality Planning and Standards. U.S. Environmental Protection Agency, Research Triangle Park, NC (2003). Available online at http://www.epa.gov/ttn/chief/conference/ei12/index.html#ses-10

Rao, S.T., J. Irwin, K. Schere, T. Pierce, R. Dennis, and J. Ching. Past, present, and future air quality modeling and its applications in the United States. *The 8th International Atmospheric Sciences and Applications to Air Quality (AASAQ 2003) Conference, March 10-13, 2003, Tsukuba, Japan*. (2003).

Rao, S.T., J.Y. Ku, S. Berman, K. Zhang, and H. Mao. Summertime characteristics of the atmospheric boundary layer and relationships to ozone levels over the eastern United States. *Pure and Applied Geophysics* 160:21-55 (2003).

Sestak, M, S. O'Neill, S. Ferguson, J. Ching, and D. G. Fox. Integration of Wildfire Emissions into the Models-3/CMAQ with the Prototypes: Community Smoke Emissions Modeling System (CSEM) and BLUESKY. In the *2002 Models-3 Users Workshop, Research Triangle Park, North Carolina, October 21-23, 2002.* Community Modeling and Analysis System (CMAS) Center, Research Triangle Park, NC (2003). Available at http://www.cmascenter.org/workshop/session5/strum_slides.ppt

Sistla, G., K. Civerolo, W. Hao, and S.T. Rao. An evaluation of the UAM-V predicted concentrations of carbon monoxide and reactive nitrogen compounds over the eastern United States. *Journal of the Air & Waste Management* 52:1324–1332 (2002).

Snyder, W.H., D.K. Heist, S.G. Perry, R. S. Thompson, and R.E. Lawson, Jr. Wind tunnel simulations to assess dispersions around the World Trade Center. In *Proceedings of PHYSMOD2003 International Workshop on Physical Modeling of Flow and Dispersion Phenomena, September 3–5, 2003, Prato, Italy.*

Stockwell, W.R., R.S. Artz, J.F. Meagher, R.A. Petersen, K.L. Schere, G.A. Grell, S.E. Peckham, A.F. Stein, R.V. Pierce, J.M. O'Sullivan, and P.Y. Whung. The scientific basis of NOAA's air quality forecasting program. EM December:20-27 (2002).

Streicher, J.J., and K. Endres. Modeling assessment of the biological and economic impact of increased UV radiation on loblolly pine in the Middle Atlantic States. In *Managing for Healthy Ecosystems*. D.J. Rapport et al. (Eds.). Lewis Publications CRC Press, Washington DC, 513-527 (2003).

Strum, M., L. Driver, G. Gipson, W.G. Benjey, R. Cook, M. Houyoux, C. Seppansen, and G. Stella. The Use of SMOKE to Process Multipollutant Inventories - Integration of Hazardous Air Pollutant and Volatile Organic Compound Emissions. In *The Twelfth International Emission Inventory Conference: Applying New Technologies, San Diego, California, April 29-May 1, 2003.* Office of Air Quality Planning and Standards. U.S. Environmental Protection Agency, Research Triangle Park, NC (2003). Available at http://www.epa.gov/ttn/chief/conference/ei12/index.html#ses-10.

Strum, M., M. Houxyoux, R. Ryan, G. Stella, W. Benjey, G. Gipson, and R. Cook. Integration of criteria and toxic pollutants in SMOKE. In *The 2002 Models-3 Users Workshop, Research Triangle Park, North Carolina, October 21-23, 2002.* Community Modeling and Analysis System (CMAS) Center, Research Triangle Park, NC (2003). Available at http://www.cmascenter.org/workshop/session5/strum_slides.ppt

Sullivan, T.J., B.J. Cosby, J.A Laurence, R.L. Dennis, K. Savig, J.R. Webb, A.J. Bulger, M. Scruggs, C. Gordon, J. Ray, E.H. Lee, W.E. Hogsett, H. Wayne, D. Miller, and J.S. Kern. *Assessment of Air Quality and Related Values in Shenandoah National Park*, Technical Report NPS/NERCHAL/NRTR-03/090, National Park Service, U.S. Department of the Interior, Northeast Region, Philadelphia, Pennsylvania, 2003.

Vickery, J. Conceptual models of PM for North American areas. R.L.Dennis (Contributing Author) Chapter 10. In *Particulate Matter Science for Policy Makers: a NARSTO Assessment*. EPRI Report No. 1007735 for NARSTO, February 2003 (2003).

Wu, Y., B. Brashers, P. L. Finkelstein and J. E. Pleim. A multilayer biochemical dry deposition model, Part 1: Model formulation. *Journal of Geophysical Research-Atmospheres* 108(D1), 4013, doi:10.1029/2002JD002293 (2003).

Wu, Y., B. Brashers, P.L. Finkelstein, and J.E. Pleim. A multilayer biochemical dry deposition model, Part 2: Model evaluation. *Journal of Geophysical Research-Atmospheres* 108(D1), 4014, doi:10.1029/2002JD002306 (2003).

Yu, S., P.S. Kasibhatla, D.L Wright, S.E. Schwartz, R. McGraw, and A. Deng. Moment-based simulation of microphysical properties of sulfate aerosols in the eastern United States: Model description, evaluation, and regional analysis. *Journal of Geophysical Research-Atmospheres* 108, No. D21, 4353, doi:10.1029/2002JDJ002890 (2003).

APPENDIX C: PRESENTATIONS

Bhave, P.V. Air pollution at the single-particle level: Integrating atmospheric measurements with mathematical models. Seminar presented at the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, June 19, 2003.

Bhave, P.V. EPA's vision for CMAQ. Presentation at the University of California, Davis, Air Quality Research Group, Davis, CA, September 8, 2003.

Ching, J.K.S. Modeling $PM_{2.5}$ with Models-3/CMAQ for exposure assessments. Presentation at the *Conference of the American Association for Aerosol Research*, Charlotte, North Carolina, October 9, 2002.

Ching, J.K.S. Subgrid air pollution concentration distributions as a complement to fine scale air quality modeling. Presentation at the *Seventh Annual Conference on Transport and Dispersion Modeling*, George Mason University, Fairfax, VA, June 17, 2003.

Cooter, E.J. Evaluation of CMAQ/atrazine results against 1995 field observations. Seminar presented at the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, November 14, 2002.

Dennis. R.L. NO_x versus VOC control for ozone attainment in the southeast United States: A combined data and CMAQ model analysis with SOS 99 surface observations. Presentation at the US-German Workshop #2—Photochemistry, Bad Breisig, Germany, October 10, 2002.

Dennis, R.L. Modeling and policy support: From RADM to CMAQ. Seminar presented at the National Institute of Public Health and the Environment, The Hague, Netherlands, October 17, 2002.

Dennis, R.L. From acidifying to eutrophying deposition: An evolving path and evolving model (from NAPAP to N2001). Presentation at the National Institute of Public Health and the Environment, The Hague, Netherlands, October 17, 2002.

Dennis, R.L. Modeling issues for PM. Presentation at the AWMA Information Exchange/ORD PM Research Panel, Research Triangle Park, NC, December 3, 2002.

Dennis, R.L. Numerical modeling of regional air quality: Lining up model and measurements to probe and address uncertainty. Invited presentation at the SAMSI/GSP Workshop on Spatio-Temporal Modeling, National Center for Atmospheric Research, Boulder, CO, June 2, 2003.

Dennis, R.L. CMAQ winter predictions of nitrate: The importance of N_2O_5 reactions in HNO_3 production. Seminar presented at the NOAA Aeronomy Laboratory, Boulder, CO, June 4, 2003.

Dennis, R.L. Model evaluation activities. Presentation at the EPA Air Program Review, Research Triangle Park, NC, September 30, 2003.

Dolwick, P.D. Plot that storm! Presentation to the Millbrook Elementary 5th grade classes (3), Raleigh, NC, October 16, 2002.

Dolwick, P.D. Science spectacular: Plot that storm! Presentation to Apex Elementary 5th grade classes (3), Apex, NC, November 22, 2002.

Dolwick, P.D. Science spectacular: Planet Polluto. Presentation to Apex Elementary 1st grade classes (3), Apex, NC, February 7, 2003.

Dolwick, P.D. Plot that storm! Presentation to Chatham Charter School 5th grade classes (2), Siler City, NC, March 28, 2003.

Dolwick, P.D. Weather safety. Presentation to Olive Chapel Elementary kindergarten classes (4), Apex, NC, April 10, 2003.

Dolwick, P.D. EPA-funded activities designed to assist Regional/State/Local Agencies with year-round air quality forecasting. Meeting on Year-Round/Multi-pollutant Air Quality Forecasting and Outreach, Research Triangle Park, NC, April 24, 2003.

Dolwick, P.D. Air quality index (AQI): Year-round forecasting. Presentation at the Spring 2003 SASWG Meeting (by phone), Baltimore, MD, May 2, 2003.

Dolwick, P.D. Monitoring the weather. Presentation to Oak Grove Elementary 2nd grade classes (4), Cary, NC, June 5, 2003.

Dolwick, P.D. Transport rule update: Ozone modeling results and issues. Presentation to the EPA Assistant Administrator for the Office of Air and Radiation, Washington DC, June 30, 2003

Dolwick, P.D. Effect of revised MCIP on modeled air quality. Presentation at the Ad Hoc Meteorological Modeling Group, Des Plaines, IL, July 29, 2003.

Dolwick, P.D. EPA-funded activities designed to assist Regional/State/Local Agencies with year-round air quality forecasting. MARAMA $PM_{2.5}$ Forecasting Meeting, Woodbridge, VA, August 12, 2003.

Dupont, S. Modeling at the neighborhood scale. Presentation at the 2002 Models-3 Users' Workshop, Research Triangle Park, NC, October 21, 2002.

Eder, B.K. Testing of the June 2002 version of the U.S. EPA's CMAQ model. Presentation at the US-German Workshop #2—Photochemistry, Bad Bresig, Germany, October 8, 2002.

Eder, B.K. An evaluation protocol for NOAA's air quality forecasting pilot program. Presentation at NOAA, Silver Spring, MD, November 7, 2002.

Eder, B.K. Operational evaluation of air quality forecast models: Protocol development. Presentation at NOAA, Silver Spring, MD, March 14, 2003.

Eder, B.K. An evaluation of the Models-3/CMAQ aerosol module. Presentation at the *2003 AAAR PM Meeting: Atmospheric Sciences, Exposures and the Fourth Colloquium on PM and Human Health*, Pittsburgh, PA, April 4, 2003.

Eder, B.K. Preliminary evaluation of the June 2002 version of CMAQ. Presentation at the 2002 Models-3 Users' Workshop, Research Triangle Park, NC, October 22, 2002.

Eder, B.K. Characterizing the spatiotemporal variability of environmental data. Presentation at the Statistical and Applied Mathematical Sciences Institute, Research Triangle Park, NC, January 24, 2003.

Fine, S.S. Introduction to EPA's Multimedia Integrated Modeling System software suite: A new framework for Models-3. Presentation at the 2002 Models-3 Users' Workshop, Research Triangle Park, NC, October 22, 2002.

Gillette, D.A. Modeling of dust emissions. Presentation at the Sino-U.S. Workshop on Dust Storm and Its Effect on Human Health, Raleigh, NC, November 25, 2002.

Gillette, D.A. Lessons on dust emissions derived from experimentation and development of a model for Owens (dry) Lake, CA, dust emissions. Presentation at the *2002 Fall Meeting of the American Geophysical Union*, San Francisco, CA, December 2002.

Gillette, D.A. Dust emissions from mesquite-vegetated sites in the Chihuahuan Dessert. Presentation at the *Jornada Symposium of the National Science Foundation's Longterm Ecological Research Project*, Las Cruces, NM, June 11, 2003.

Gilliland, A.B. Community Multiscale Air Quality modeling: Global climate change and air quality. Presentation at the EPA STAR Kickoff Meeting for 2002 Climate and Air Quality Grants, Research Triangle Park, NC, March 23, 2002.

Gipson, G.L. Improvements to the computational efficiency of modeling gas-phase chemistry in CMAQ. Seminar presented at the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, February 27, 2003.

Godowitch, J.M. Photochemical and aerosol modeling with the CMAQ Plume-in-Grid approach. Seminar presented at the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, September 25, 2003.

He, S. Modeling fugitive dust in the United States with the Models-3/Community Multiscale Air Quality modeling system. Presentation at the *Conference of the American Association for Aerosol Research*, Charlotte, North Carolina, October 10, 2002.

He, S. Development of a windblown fugitive dust emission model with the Models-3/Community Multiscale Air Quality modeling system. Presentation at the 2002 Models-3 Users' Workshop, Research Triangle Park, NC, October 22, 2002.

Heist, D.K. Wind tunnel simulations to assess dispersion around the World Trade Center. Presentation at the *PHYSMOD2003: International Workshop on Physical Modeling of Flow and Dispersion Phenomena*, Prato, Italy, September 4, 2003.

Huber, A.H. Visualization and simulation of toxic air pollutants released in urban areas—Including homeland security applications. Presentation at the 2002 SGI Homeland Security Summit, Washington DC, November 13, 2002.

Huber, A.H. Environmental CFD simulation and visualization: Examples in support of the reconstruction of the smoke/dust plume from the World Trade Center site following the events of September 11, 2001. Poster presentation at the EPA Science Forum, Washington, DC, May 5-6, 2003.

Huber, A.H. A New York World Trade Center project: Before, during, and after September 11, 2001. Seminar presented at the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, August 21, 2003.

Huber, A.H. Evaluation of potential human exposures and health impacts of airborne particulate matter (PM) and its constituents following the collapse of the World Trade Center towers. Presentation at the American Chemical Society Meeting, New York, NY, September 11, 2003.

Hutzell, W.T. A regional model for PCDD/F's based on a photochemical model for air quality and particulate matter. Presentation at the *2002 Fall Meeting of the American Geophysical Union*, San Francisco, CA, December 6, 2002.

Irwin, J.S. Application of ASTM D6589 to evaluate dispersion model performance to simulate average centerline concentration values. Presentation at the *8th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*, Sofia, Bulgaria, October 15, 2002.

Luecken, D.J. Regional scale assessments and the atmospheric fate and transport of air toxics: CMAQ. Presentation at the Risk Assessment Modeling Tools Symposium, Chicago, Illinois, July 16, 2003.

Luecken, D.J. Predicting the atmospheric fate and transport of air toxics using CMAQ. Seminar presented at the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, July 31, 2003.

Luecken, D.J. Modeling the atmospheric concentrations of toxic air pollutants. Presentation at the U.S. EPA's National Exposure Research Laboratory Air Research Program Peer Review, Research Triangle Park, NC, September 30, 2003.

Otte, T.L. Science fair data presentation techniques. Presentation to 5^{th}-grade classes (3) at Olive Chapel Elementary School, Apex, NC, February 7, 2003.

Otte, T.L. Weather basics: Evaporation and condensation. Presentation to 2^{nd}-grade class at Morrisville Elementary School, Morrisville, NC, March 28, 2003.

Otte, T.L. Recent changes in MCIP2. Seminar presented at the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, May 8, 2003.

Perry, S.G. Simulation and visualization of the smoke/dust plume from the World Trade Center site. Presentation at the U.S. Environmental Protection Agency Science Fair, Washington, DC, May 6, 2003.

Pierce. T.E. Biogenic emissions: Is the uncertainty growing? Presentation at the U.S.-German Workshop, *Ozone and Particles: Policy and Science—Recent Developments and Controversial Issues (Regional and Urban Air Pollution)*, Bad Breisig, Germany, October 10, 2002.

Pleim, J.E. Future enhancements of the CMAQ model. Presentation at the 2003 Models-3 Users' Workshop, Research Triangle Park, NC, October 22, 2003.

Pouliot, G.A. Advances in emissions modeling of airborne substances. Poster presentation at *the* 12^{th} *International Emission Inventory Conference, "Emission Inventories—Applying New Technologies*," San Diego, California, April 28, 2003.

Pouliot, G.A. Creating an emission inventory for modeling global climate change effects on regional air quality. Presentation at *the 12th International Emission Inventory Conference, "Emission Inventories—Applying New Technologies*," San Diego, California, April 28, 2003.

Pouliot, G.A. Emissions processing for an air quality forecasting model. Poster presentation at *the 12th International Emission Inventory Conference, "Emission Inventories—Applying New Technologies*," San Diego, California, April 28, 2003.

Rao, S.T. Using regional-scale photochemical models for guiding emissions management decisions. Presentation at the U.S.-German Workshop, *Ozone and Particles: Policy and Science—Recent Developments and Controversial Issues (Regional and Urban Air Pollution)*, Bad Breisig, Germany, October 9, 2002.

Rao, S.T. Past, present, and future air quality modeling and its applications in the United States. Presentation at the *International Conference on Atmospheric Sciences and Applications to Air Quality (ASAAQ)*, Tsukuba Science City, Japan, March 11, 2003.

Rao, S.T. Comparison of the space-time signatures of air quality data from different networks. Presentation at the *NATO-CCMS International technical Meeting on Air Pollution Modeling and Its Applications*, Istanbul, Turkey, May 28, 2003.

Roselle, S.J. CMAQ briefing to the U.S. EPA's Office of Air Quality Planning and Standards. Research Triangle Park, NC, March 27, 2003.

Russell, O.R., Jr. Mercury emissions and atmospheric transport, mercury TMDLs: Science and model building, modeling mercury deposition. Western Mercury Workshop, EPA Region 8, Denver, CO, April 22, 2003.

Russell, O.R. Jr. Atmospheric mercury models: What can they tell us about air transport and fate? Presentation at the Society of Environmental Toxicology and Chemistry Mercury Workshop, Pensacola, FL, September 15, 2003.

Schere, K.L. The Models-3/CMAQ model: 2002 release - new features. Presentation at the 2002 Models-3 Users' Workshop, Research Triangle Park, NC, October 21, 2002.

Schere, K.L. The EPA CMAQ modeling system. Presentation at the NOAA/NWS/OAR Air Quality Forecasting Workshop, Silver Spring, MD, November 7, 2002.

Schere, K.L. NOAA air quality forecast modeling program. Presentation at the *U.S. EPA/AWMA 2003 National Air Quality Conference*, San Antonio, TX, February 4, 2003.

Schere, K.L. NOAA air quality forecast modeling project. Seminar presented at the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, February 20, 2003.

Schere, K.L. The U.S. EPA Community Multiscale Air Quality modeling system - Current status and applications. Presentation at the Atmospheric Sciences and Applications to Air Quality (ASAAQ)-2003 Conference, Tsukuba, Japan, March 13, 2003.

Schere, K.L. NOAA/EPA operational air quality forecast model system. Presentation at the Planning Meeting for Summer 2004 Climate and Air Quality Field Campaign, Durham, NH, April 23, 2003.

Schere, K.L. CMAQ research update: Nitrate overprediction, optimization, secondary organic aerosol. Presentation for the U.S. EPA, Office of Air Quality and Planning Standards, Research Triangle Park, NC, July 8, 2003.

Schere, K.L. Meteorological and atmospheric modeling—Model development. Presentation at the U.S. EPA's National Exposure Research Laboratory Air Research Program Peer Review, Research Triangle Park, NC, September 30, 2003.

Schwede, D.B. Use of magnets for navigation, Franciscan School, Raleigh, NC, October 21, 2002.

Young, J.O. Recent developments for parallel CMAQ. Seminar presented at the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, July 24, 2003.

Yu, S. Primary and secondary organic aerosols over the United States: Estimates on the basis of observed organic carbon (OC) and elemental carbon (EC), and air quality modeled primary OC/EC ratios. Presentation at the 2003 Models-3 Users' Workshop, Research Triangle Park, NC, October 23, 2003.

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Yu, S. Simulation of primary and secondary (biogenic and anthropogenic) organic aerosols over the United States by U.S. EPA Models-3/CMAQ: Evaluation and regional analysis. Presentation at the 2003 Models-3 Users' Workshop, Research Triangle Park, NC, October 23, 2003.

Yu, S. Relative contributions of primary and secondary (biogenic and anthropogenic) organic aerosols at Nashville: Comparisons of observations and modeling results. Presentation at the *2003 AAAR PM Meeting: Atmospheric Sciences, Exposure and the Fourth Colloquium on PM and Human Health*, Pittsburgh, PA, April 1, 2003.

Yu, S. Primary and secondary organic aerosols over the United States: Estimates on the basis of observations and modeled primary OC/EC ratios. Presentation at the *2003 AAAR PM Meeting: Atmospheric Sciences, Exposures and the Fourth Colloquium on PM and Human Health*, Pittsburgh, PA, April 2, 2003.

Yu, S. Simulation of primary and secondary (biogenic and anthropogenic) organic aerosol over the Unites States by U.S. EPA Models-3/CMAQ: Evaluation and regional analysis. Presentation at the EGS-AGU-EUG Joint Assembly, Nice, France, April 10, 2003.

Yu, S. Can the thermodynamic model and 3-D air quality model predict the aerosol NO_3- reasonably within a factor of 2? Presentation at the 2003 Models-3 Users' Workshop, Research Triangle Park, NC, October 23, 2003.

Yu, S. New unbiased symmetric metrics for evaluation of air quality model. Presentation at the 2003 Models-3 Users' Workshop, Research Triangle Park, NC, October 23, 2003.

APPENDIX D: WORKSHOPS AND MEETINGS

Methyl Mercury Interagency Working Group, Washington, DC, October 2, 2002.

O.R. Bullock, Jr.

US-German Workshops on Photochemistry and Intercontinental Transport, Bad Breisig, Germany, October 7–11, 2002.

R.L. Dennis	T.E. Pierce
B.K. Eder	S.T. Rao

VISTAS Fire Emission Workshop, Research Triangle Park, NC, October 17, 2002.

W.G. Benjey

2002 Models-3 User's Workshop, Research Triangle Park, NC, October 21–23, 2002..

D.A. Atkinson	B.K. Eder	He, S	G. Pouliot .
W.G. Benjey	M.L. Evangelista	J.S. Irwin	S.J. Roselle
J.K.S. Ching	S.S. Fine	T.L. Otte	K.L. Schere
R.L. Dennis	G.L. Gipson	T.E. Pierce	J.L. Young
P.D. Dolwick	J.M. Godowitch	J.E. Pleim	

NOAA Air Quality Forecast Workshop, Silver Spring, MD, November 7–8, 2002.

B.K. Eder	S.T. Rao
T.E. Pierce	K.L. Schere
J.E. Pleim	

TARC Proposal Review Panel, Houston, TX, November 11–12, 2002.

R.L. Dennis

Sino-U.S. Workshop on Dust Storms and its Effect on Human Health, Raleigh, NC, November 25–26, 2002.

D.A. Gillette

AWMA Information Exchange/ORD PM Research Panel, Research Triangle Park, NC, December 3–4, 2002.

R.L. Dennis

U.S. Climate Change Science Program: Planning Workshop for Scientists and Stakeholders, Washington, DC, December 3–5, 2002.

K.L. Schere

Methyl Mercury Interagency Working Group, Washington, DC, December 6, 2002.

O.R. Bullock, Jr.

American Geophysical Union 2002 Fall Meeting, San Francisco, CA, December 6–10, 2002.

D.A. Gillette
W.T. Hutzell

Air Resource Laboratory Transport Dispersion Modeling Meeting, Washington, DC, December 10, 2002.

A.H. Huber

EPA's 2003 National Air Quality Conference: Its Not Just About Ozone Anymore, San Antonia, TX, February 2–5, 2003.

P.D. Dolwick
B.K. Eder
K.L. Schere

BRACE Workshop, Tampa Bay, FL, February 3–4, 2003.

R.L. Dennis

BRACE Aerosol Meeting, University of South Florida, College of Public Health, Tampa Bay, FL, February 5, 2003.

R.L. Dennis

Annual Meeting of the American Meteorological Society, Long Beach, CA, February 9–13, 2003.

E.M. Poole-Kober

Sixth Conference of Atmospheric Librarians International, Long Beach, CA, February 12–14, 2003.

E.M. Poole-Kober

Columbia University Climate and Health Project Meeting, New York, NY, February 26–27, 2003.

K.L. Schere

Second Workshop on Air Quality Modeling, Tsukuba, Japan, March 10, 2003.

S.T. Rao
K.L. Schere

EPA STAR Kickoff Meeting for 2002 Climate and Air Quality Grants, Research Triangle Park, NC, March 23, 2002.

A.B. Gilliland

Great Lakes Regional Mercury Monitoring Workshop, East Lansing, MI, March 26–27, 2003.

O.R. Bullock, Jr.

Eleventh Jet Propulsion Lab Airborne Earth Science Workshop, Pasadena, CA, March 31–April 2, 2003.

J.J. Streicher

American Association for Aerosol Research Conference, PM Meeting: Atmospheric Sciences, Exposures and the Fourth Colloquium on PM and Human Health, Pittsburgh, PA, March 31–April 4, 2003.

R.L. Dennis, Co-Chair
B.K. Eder
J.M. Godowitch
W.T. Hutzell
M.R. Mebust

NOAA/National Centers for Environmental Prediction Air Quality Forecast Meeting, Silver Springs, MD, April 15, 2003.

K.L. Schere

Western Mercury Workshop, EPA Region 8, Denver, CO, April 21–22, 2003.

O.R. Bullock, Jr.

Planning Meeting for Summer 2004 Climate and Air Quality Field Campaign, Durham, NH, April 22–23, 2003.

R.L. Dennis
K.L. Schere

Meeting on Year-Round/Multi-pollutant Air Quality Forecasting and Outreach, Research Triangle Park, NC, April 24, 2003.

P.D. Dolwick

12th International Emission Inventory Conference, "Emission Inventories—Applying New Technologies," San Diego, California, April 28–May 1, 2003.

J.D. Mobley, Chair, Poster Session
G.A. Pouliot

Waterloo Centre for Atmospheric Sciences Meeting, University of Waterloo, Waterloo, Canada, April 29–30, 2003.

K.L. Schere
S.T. Rao

Workshop on Air Quality Forecasting, U.S Weather Research Program Office, Houston, Texas, April 29–May 2, 2003.

J.K.S. Ching

Technical Meeting on Air Quality Forecasting, National Centers for Environmental Predictions, Camp Springs, MD, May 1, 2003.

T.L. Otte

EPA 2003 Science Forum, Washington, DC, May 5–7, 2003.
A.H. Huber
K.L. Schere

SAIL (Southeast Affiliate of IAMSLIC Librarians) 2003 Annual Meeting, Harbor Branch Oceanographic Institution, Fort Pierce, FL, May 13–16, 2003.

E.M. Poole-Kober

26th NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Istanbul, Turkey, May 19–23, 2003.

S. Dupont

SAMSI/GSP Workshop on Spatio-Temporal Modeling, National Center for Atmospheric Research, Boulder, CO, June 1–6, 2003.

R.L. Dennis

MM5/WRF 3DVAR Tutorial, Boulder, CO, June 9, 2003.
R.C. Gilliam
J.E. Pleim

MM5/WRF Workshops, Boulder, CO, June 10–13, 2003.
R.C. Gilliam
J.E. Pleim

Workshop on Wildland Fire Emissions Modeling, U.S. Forest Service, Seattle, Washington, June 11–12, 2003.

T.E. Pierce

NOAA Data User's Workshop, Boulder, CO, June 11–13, 2003.

D.A. Atkinson

Air Quality Modeling Meeting of Chesapeake Bay Program, NOAA Chesapeake Bay Program Office, Annapolis, MD, June 16, 2003.

R.L. Dennis

Seventh Annual George Mason University Transport and Dispersion Modeling Conference, Fairfax, Virginia, June 17–19, 2003.

J.K.S. Ching
S.G. Perry

R.S. Thompson

1st World Congress on Risk, Brussels, Belgium, June 20-27, 2003.

A.H. Huber

Air & Waste Management Association 96th Annual Conference, San Diego, California, June 22–26, 2003.

D.A. Gillette

Thirty First Annual Meeting of the American Society for Photobiology, Baltimore, MD, July 5–9, 2003.

J.J. Streicher

Air Toxic Risk Assessment Modeling Tools Symposium; Chicago, IL, July 15–17, 2003.

D.J. Luecken

NOAA/OAR Air Quality Forecast Planning Meeting, Boulder, CO, July 21, 2003.

S.S. Fine
J.E. Pleim
S.J. Roselle
K.L. Schere

Air Quality Meeting, National Center for Atmospheric Research, Boulder, CO, July 21, 2003.

S.J. Roselle

Ad Hoc Meteorological Modeling Group, Des Plaines, IL, July 29, 2003.

P.D. Dolwick

Joint Statistical Meetings 2003, Session, Applications in Spatio-Temporal Modelling: From the F-22 to fMRI, San Francisco, CA, August 3, 2003.

J.L. Swall, Chair

Managing Safety: Systems that Work for Senior Leader, Silver Spring, MD, August 3–6, 2003.

K.L. Schere

MARAMA $PM_{2.5}$ Forecasting Meeting, Woodbridge, VA, August 12, 2003.

P.D. Dolwick

Workshop on Uncertainties in Emissions Modeling, American Petroleum Institute, Houston, Texas, August 26–27, 2003.

W.G. Benjey

Air Resources Laboratory Climate Coordination Meeting, Silver Springs, Maryland, August 28, 2003.

E.J. Cooter
J.J. Streicher

PHYSMOD2003: International Workshop on Physical Modeling of Flow and Dispersion Phenomena, Prato, Italy, September 3–5, 2003.

D.K. Heist

National Science Foundation Review of Long Term Ecological Research Project at Jornada LTER, Las Cruses, NM, September 8–10, 2003.

D.A. Gillette

EMEP Steering Body Meeting, Geneva, Switzerland, September 8–11, 2003.

R.L. Dennis

$PM_{2.5}$ Forecasting Workshop: Southeastern United States, Research Triangle Park, NC, September 11–12, 2003.

P.D. Dolwick

$PM_{2.5}$ Forecasting Workshop: Midwestern United States, Des Plaines, IL, September 15–16, 2003.

P.D. Dolwick

International Standards Organization (ISO) Technical Committee 146 Subgroup Week, Bautahoj Kursuscenter, Jaegerspris, Denmark, September 21–25, 2003.

J.S. Irwin

EPA Air Program Review, Research Triangle Park, NC, September 29–30, 2003.

R.L. Dennis
K.L. Schere

NOAA Air Quality Forecast Focus Group Meeting, Silver Spring, MD, September 9–10, 2003.

J.E. Pleim
K.L. Schere

Third Russian Mercury Emission Inventory Workshop of the Arctic Monitoring and Assessment Program, Moscow, Russia, September 10–11, 2003.

O.R. Bullock, Jr.

Mercury Science Workshop, Pensacola, FL, September 14–17, 2003.

O.R. Bullock, Jr.

Air Quality IV Conference, Arlington, VA, September 23–24, 2003.

K.L. Schere

APPENDIX E: VISITING SCIENTISTS

Dr. Daewon Byun, Jiwen He, and Joshua Fu
Department of Geosciences
University of Houston
312 Science & Research, Building 1
Houston, TX 77204

Dr. Byun, He, and Fu visited the Division on January 10, 2003, to present seminars on air quality research at the University of Houston.

Dr. David Rogers, Dr. Jack Hayes, Dr. Nelson Seaman, and Dr. Paula Davidson
NOAA/National Weather Service
Silver Spring, MD

Drs. Rogers, Hayes, Seaman, and Davidson visited the Division on January 30, 2003, to attend a meeting on the NOAA/EPA collaboration on air quality forecasting.

Dr. Nelson Seaman
Department of Meteorology
Pennsylvania State University
503 Walker Building
University Park, PA 16802

Dr. Seaman visited the Division on January 7, 2003, to participate in discussions on the NOAA/EPA collaboration on air quality forecasting.

Sue Stendebach
National Science Foundation
Arlington, Virginia

Ms. Stendebach visited the Division on May 1, 2003, to discuss the Digital Government Research program of NSF.

Dr. Stephen E. Schwartz
Brookhaven National Laboratory
Upton, NY

Dr. Stephen E. Schwartz visited the Division on August 4, 2003, to present a seminar on aerosols and climate change.

Jim Tuccillo
IBM Corporation
Atlanta, GA

Mr. Tuccillo visited the Division on February 20 and March 24, 2003, to discuss CMAQ model code optimization for air quality forecasting.

Dr. Satoshi Yamazaki (Toyota Research)
Dr. Hitoshi Kunimi (Nissan Research),
Mr. Yoshiaki Shibata (Petroleum Energy Center)
Mr. Tatsuo Omata (Petroleum Energy Center)
Mr. Tetsuji Watanabe (Petroleum Energy Center)
Japan Clean Air Program
Tokyo, Japan

Drs. Yamazaki, and Kunimi, and Messrs. Shibata, Omata, and Watanabe visited the Division on July 21–22, 2003, to discuss collaboration on CMAQ modeling in the United States and Japan.

APPENDIX F: POSTDOCTORAL RESEARCHERS

Dr. Sylvain Dupont performed research as an UCAR post-doc to integrate refined Urban Canopy Parameterizations (UCPs) in the meteorological model MM5. This advanced version of MM5 should improve the simulation of turbulence and transport fields within and above the urban and vegetative canopies for more accurate fine-scale simulations with the Community Multiscale Air Quality (CMAQ) modeling system in urban areas.

Sylvain Dupont worked on an urban canopy parameterization for the MM5 meteorological model to better simulate turbulence and energy exchanges within urban areas.

Shaocai Yu conducted research on CMAQ model diagnostic evaluation of PM2.5 and its components, including comprehensive sensitivity and assessment testing of the aerosol thermodynamic partitioning scheme.

Daiwen Kang worked on model evaluation procedures for the emerging NOAA air quality forecast capability, including evaluation of several pilot model platforms for ozone forecasting.

APPENDIX G: ATMOSPHERIC SCIENCES MODELING DIVISION STAFF AND AWARDS

All personnel are attached to the Environmental Protection Agency from the National Oceanic and Atmospheric Administration, except those designated EPA, who are employees of the Environmental Protection Agency, or SEEP, who are part of the EPA Senior Environmental Employment Program.

Office of the Director

Dr. S.T. Rao, Supervisory Meteorologist, Director
J. David Mobley (EPA), Environmental Engineer, Associate Director
William B. Petersen, Physical Science Administrator, Assistant Director
Dr. Jay Messer (EPA), Physical Scientist
Jeffrey L. West, Physical Science Administrator
Barbara R. Hinton (EPA), Secretary

Program Operations Staff

Herbert J. Viebrock, Supervisory Physical Scientist, Chief
Linda W. Green, Administrative Specialist
Evelyn M. Poole-Kober, Librarian
John H. Rudisill, III, Equipment Specialist

Atmospheric Model Development Branch

Kenneth L. Schere, Supervisory Meteorologist, Chief
Dr. Prakash V. Bhave, Physical Scientist (Since March 2003)
O. Russell Bullock, Meteorologist
Gerald L. Gipson (EPA), Physical Scientist
Robert C. Gilliam, Meteorologist (Since April 2003)
James M. Godowitch, Meteorologist
Dr. Alan H. Huber, Physical Scientist
Dr. William T. Hutzell (EPA), Physical Scientist
Dr. Michelle R. Mebust (EPA), Physical Scientist (Until August 2003)
Tanya L. Otte, Meteorologist
Dr. Jonathan E. Pleim, Physical Scientist
Shawn J. Roselle, Meteorologist
Dr. Jeffrey O. Young, Mathematician
Patricia F. McGhee, Secretary

Model Evaluation and Applications Research Branch

Dr. Steven S. Fine, Supervisory Physical Scientist, Chief
Dr. Robin L. Dennis, Physical Scientist
Dr. Brian K. Eder, Meteorologist
Dr. Peter L. Finkelstein, Physical Scientist
Dr. Alice B. Gilliland, Physical Science Administrator
Steven C. Howard, IT Specialist
Dr. Jenise L. Swall, Statistician (Since June 2003)
Alfreida R. Torian, IT Specialist
Gary L. Walter, Computer Scientist
Sherry A Brown, Secretary

Air-Surface Processes Modeling Branch

Thomas F. Pierce, Supervisory Physical Scientist, Chief
Dr. William G. Benjey, Physical Scientist
Dr. Jason K.S. Ching, Meteorologist
Dr. Ellen J. Cooter, Meteorologist
Dr. Dale A. Gillette, Physical Scientist
Dr. David K. Heist, Physical Scientist (Since August 2003)
Dr. Steven G. Perry, Meteorologist
Dr. George A. Pouliot, Physical Scientist
Donna B. Schwede, Physical Scientist
John J. Streicher, Physical Scientist
Roger S. Thompson, Physical Scientist (Until September 2003)
Bruce Pagnani (SEEP), Computer Programmer
Ashok Patel (SEEP), Engineer
John Rose (SEEP), Machinist/Modeler
Ruby Borden (SEEP), Secretary (Until January 2003)
Jane Coleman (SEEP), Secretary (Since March 2003)

Air Policy Support Branch

Mark L. Evangelista, Supervisory Meteorologist, Chief
Dennis A. Atkinson, Meteorologist
Dr. Desmond T. Bailey, Meteorologist
Patrick D. Dolwick, Physical Scientist
John S. Irwin, Meteorologist
Brian L. Orndorff, Meteorologist
Jawad S. Touma, Meteorologist

Awards

Dennis Atkinson, Dr. Desmond Bailey, and John Irwin received EPA Bronze Medals for superior customer service to the air quality community.

Mark Evangelista received an EPA Bronze Medal for initiative, creativity, and dedicated work in community outreach.